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FILE COVERS 1907 - 6 Dec 2004 VOL 141 ISS 24 FILE LAST UPDATED: 5 Dec 2004 (20041205/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> => d stat que 120 L7 STR

O 7 C G2 C G4

0 9 10 @11 12

1 C G1

6 C 5 G3 4

VAR G2=ME/OH/MEO
VAR G3=CH/11
VAR G4=OH/ME/MEO/NO2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

VAR G1=CH/9

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE L9 SCR 1839

L11 4180 SEA FILE=REGISTRY SSS FUL L7 NOT L9

L14 STI

VAR G1=CH/9
VAR G2=ME/OH/MEO
VAR G3=CH/11
VAR G4=OH/ME/MEO/NO2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

T<sub>1</sub>19

L20

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L15 901 SEA FILE=REGISTRY SUB=L11 SSS FUL L14
L16 16802 SEA FILE=HCAPLUS ABB=ON PLU=ON L15
L18 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L)(?PORIFER? OR ?HELMINTH?

OR ?COELOMA? OR ?ANNELID? OR ?WORM? OR ?MOLLUSK? OR ?BIVAL?

OR ?LARV? OR ?COPEPOD? OR ?OSTRACOD? OR ?MYSID? OR ?GAMMARID?

OR ?DECAPOD? OR ?TELEOS? OR ?STARFISH?)

361 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L)(PEST? OR AQUACID? OR ?VIRUS? OR ?PROTI? OR ?FUNGI? OR MOLD OR MOLDS OR ANTIMOLD OR ?PLANKTON? OR ?DEMERS? OR ?BENTHI? OR ?BIOTA? OR ?BACTER? OR ?PROTOZO? OR ?ALGAE? OR ?PYRROP? OR ?CRYPTOP? OR ?CHRYSOPH?)

44 SEA FILE=HCAPLUS ABB=ON PLU=ON (L18 OR L19) AND (WATER OR

AQUA?)

=> d ibib abs hitstr l20 1-44

L20 ANSWER 1 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2004:69248 HCAPLUS

DOCUMENT NUMBER:

141:20201

TITLE:

Microbial anaerobic demethylation and dechlorination

of chlorinated hydroquinone metabolites synthesized by

basidiomycete fungi

Sowers, K. R.; May, H. D.

AUTHOR(S):

Milliken, C. E.; Meier, G. P.; Watts, J. E. M.;

Department of Microbiology and Immunology, Medical

CORPORATE SOURCE:

University of South Carolina, Charleston, SC, USA
Applied and Environmental Microbiology (2004), 70(1),

SOURCE: Applied 385-392

CODEN: AEMIDF; ISSN: 0099-2240

PUBLISHER:

American Society for Microbiology

DOCUMENT TYPE:

LANGUAGE:

Journal English

AB The synthesis and degradation of anthropogenic and natural organohalides are

the basis of a global halogen cycle. Chlorinated hydroquinone metabolites (CHMs) synthesized by basidiomycete fungi and present in wetland and forest soil are constituents of that cycle. Anaerobic dehalogenating bacteria coexist with basidiomycete fungi in soils and sediments, but little is known about the fate of these halogenated fungal compds. In sediment microcosms, the CHMs 2,3,5,6-tetrachloro-1,4-dimethoxybenzene and 2,3,5,6-tetrachloro-4-methoxyphenol (TCMP) were anaerobically demethylated to tetrachlorohydroquinone (TCHQ). Subsequently, TCHQ was converted to trichlorohydroquinone and 2,5-dichlorohydroquinone (2,5-DCHQ) in freshwater and estuarine enrichment cultures. Screening of several dehalogenating bacteria revealed that Desulfitobacterium hafniense strains DCB2 and PCP1, Desulfitobacterium chlororespirans strain Co23, and Desulfitobacterium dehalogenans JW/DU1 sequentially dechlorinate TCMP to 2,3,5-trichloro-4-methoxyphenol and 3,5-dichloro-4-methoxyphenol (3,5-DCMP). After a lag, these strains demethylate 3,5-DCMP to 2,6-DCHQ, which is then completely dechlorinated to 1,4-dihydroquinone (HQ). 2,5-DCHQ accumulated as an intermediate during the dechlorination of TCHQ to HQ by the TCMP-degrading desulfitobacteria. HQ accumulation following TCMP or TCHQ dechlorination was transient and became undetectable after 14 days, which suggests mineralization of the fungal compds. This is the first report on the anaerobic degradation of fungal CHMs, and it establishes a fundamental role for microbial reductive degradation of natural organochlorides in the global halogen cycle.

IT 106-51-4, Quinone, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study) (microbial anaerobic demethylation and dechlorination of chlorinated hydroquinone metabolites synthesized by basidiomycete **fungi**)

106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

RN

CN

REFERENCE COUNT:

52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:617123 HCAPLUS

DOCUMENT NUMBER:

139:165586

TITLE:

Porous (meth)acrylic resin material with open cells

and manufacture of the material

INVENTOR(S):

Misumi, Yoshifumi; Kasahara, Shingo

PATENT ASSIGNEE(S):

Toto Ltd., Japan

Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003226709	A2	20030812	JP 2002-30869	20020207
PRIORITY APPLN. INFO.:			JP 2002-30869	20020207
and the second of the second		taad bee assast	na of a composition so	

AB The material is that obtained by curing of a composition containing water , a surfactant, a polymerization initiator, a crosslinking accelerator, an acrylic monomer, and an organic filler mixture of ≥1 selected from a (meth)acrylic monomer homopolymer, copolymers, and their crosslinked

products. The material is manufactured by the process involving (a) mixing of the components for providing of an emulsion slurry, (b) applying of the slurry into a water-nonpermeable mold, (c) demolding of the cured slurry, and (d) removing of residual aqueous solution from the cured product by pressurized air and water. Thus, an emulsion containing 520 parts poly(Me methacrylate) (Hipearl D 100M), 156 parts Me methacrylate, polyoxyethylene nonylphenyl ether (Emulgen 930), EtOH, Bz202, and N,N-dimethylaniline was molded to give a test piece, in which a slurry corresponding to a ceramic sanitary wear could be cast under only suction without pressure.

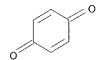
106-51-4, p-Benzoquinone, uses IT

RL: CAT (Catalyst use); USES (Uses)

(polymerization inhibitor; for preparation of porous (meth)acrylic resin material with open cells containing organic fillers for ceramic casting mold)

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CN

L20 ANSWER 3 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

2003:108822 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

139:311796

TITLE:

Bioluminescent bioassays based on luminous bacteria

marker system

AUTHOR(S):

SOURCE:

Kuznetsov, A. M.; Rodicheva, E. K.; Medvedeva, S. E.;

Gitelson, J. I.

CORPORATE SOURCE:

Institute of Biophysics, Russian Academy of Sciences,

Siberian Branch, Krasnoyarsk, 660036, Russia Bioluminescence & Chemiluminescence: Progress &

Current Applications, [Proceedings of the Symposium on

Bioluminescence and Chemiluminescence], 12th, Cambridge, United Kingdom, Apr. 5-9, 2002 (2002), 323-326. Editor(s): Stanley, Philip E.; Kricka, Larry

J. World Scientific Publishing Co. Pte. Ltd.:

Singapore, Singapore.

CODEN: 69DPGZ; ISBN: 981-238-156-2

DOCUMENT TYPE:

Conference English LANGUAGE:

Two bioluminescent bioassays based on lyophilized marine luminous bacteria, Microbiosensor B17-677F, and genetically modified luminous strain of Escherichia coli, Microbiosensor-ECK, were employed to detect zone of impaired water quality in the river and sewage water of different regions of Siberia. Effect of model substances on Microbiosensor B17-677F compared to its effect on Microbiosensor-ECK

showed that in the concentration range evaluated, dependence on the concentration of

the

substance was the same. The sensitivity of phenol compds. of the newly developed Microbiosensor-ECK was higher compared to that of Microbiosensor B17-677F. The toxicity of series of phenol compds. produced by Microbiosensor-ECK was in agreement with the toxicity series of phenol compds. determined on intact cells of Photobacterium phosphoreum luminous bacteria and various hydrobionts.

106-51-4, 2,5-Cyclohexadiene-1,4-dione, analysis TI '

RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)

(bioluminescent bioassays based on luminous bacteria marker

system for anal. of river and sewage water)

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 8

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:42826 HCAPLUS

DOCUMENT NUMBER:

138:68343

TITLE:

Biocidal compositions for controlling populations of

aquatic pest organisms containing quinones,

anthraquinones, and naphthalenediones

INVENTOR (S):

Cutler, Stephen J.; Cutler, Horace G.; Wright, David;

Dawson, Rodger

PATENT ASSIGNEE(S):

Aquacide and Use, USA

SOURCE:

U.S. Pat. Appl. Publ., 9 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003012804	A1	20030116	US 2001-886621	20010622
PRIORITY APPLN. INFO.:			US 2001-886621	20010622
4 = 3				

OTHER SOURCE(S): MARPAT 138:68343

Target aquatic pest organism populations are controlled by exposing the target population to an effective amount of (a) a biocidal compds. selected from the group consisting of quinones, anthraquinones, naphthalenediones, quinine, warfarin, coumarins, amphotalide, cyclohexadiene-1,4-dione, phenindione, pyridone, sodium rhodizonate, spirulosin and thymoquinone, and (b) a peroxy compound The method is particularly effective for treating ballast water of ships or other enclosed vols. of water subject to transport between or among geog. areas to control the relocation of plants, toxic bacteria, and animals contained in the water.

106-51-4D, Cyclohexadiene-1,4-dione, mixts. with peroxy compds. TT

319-89-1D, Tetrahydroxy-p-benzoquinone, mixts. with peroxy compds.

479-22-1D, mixts. with peroxy compds. 484-89-9D,

3-Hydroxy-2-methoxy-5-methyl-p-benzoquinone, mixts. with peroxy compds.

530-55-2D, mixts. with peroxy compds. 553-97-9D, mixts. with peroxy compds. 605-94-7D, mixts. with peroxy compds.

RL: BSU (Biological study, unclassified); BUU (Biological use,

unclassified); BIOL (Biological study); USES (Uses)

(biocidal compds. for controlling populations of aquatic

pest organisms containing)

RN 106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

RN 319-89-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy- (9CI) (CA INDEX NAME)

RN 479-22-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3,6-dinitro- (9CI) (CA INDEX NAME)

RN 484-89-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)

RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)

RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)

RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)

L20 ANSWER 5 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:42257 HCAPLUS

DOCUMENT NUMBER:

138:106698

TITLE:

Preparation of 4-arylquinols and analogs thereof as

antiproliferative agents, anticancer agents,

antimycobacterial agents, antituberculosis agents, and/or thioredoxin/thioredoxin reductase inhibitors Stevens, Malcolm Francis Graham; Wells, Geoffrey;

INVENTOR(S):

Westwell, Andrew David; Poole, Tracey Dawn

PATENT ASSIGNEE(S):

Cancer Research Technology Limited, UK PCT Int. Appl., 180 pp.

SOURCE:

CODEN: PIXXD2

Patent

DOCUMENT TYPE:

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	rent :	NO.			KIN	<b>)</b>	DATE		i	APPL	ICAT	ION 1	NO.		D	ATE	
WO	2003	0044	79		A1		2003	0116	1	WO 2	002-0	GB30	97		2	0020	705
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BΖ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	ΙL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KΖ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NΖ,	OM,	PH,
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,
		ТJ,	TM														
	RW:	GH,	GM,	KΕ,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	ВG,
		CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,
		PT,	SE,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,
		NΕ,	SN,	TD,	TG												
EP	1404	659			A1		2004	0407		EP 2	002-	7455	85		2	0020	705
	R:	AT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	SK		
JP 2004533486		T2		2004	1104		JP 2	003-	5106	46		2	0020	705			

US 2004220236 PRIORITY APPLN. INFO.:

A1 20041104

US 2004-482912

20040427 20010706

PRIORITI ATTEN: 1

GB 2001-16594 WO 2002-GB3097

W 20020705

OTHER SOURCE(S):

MARPAT 138:106698

GT

$$Q = \begin{array}{c} R^2 & R^3 \\ Ar \\ OR^1 \\ R^6 & R^5 & I \end{array}$$

$$\mathsf{Me} = \left( \begin{array}{c} \mathsf{N} \\ \mathsf{SO}_2 - \mathsf{N} \end{array} \right) = \left( \begin{array}{c} \mathsf{N} \\ \mathsf{O} \\ \mathsf{S} \\ \mathsf{Me} \end{array} \right)$$

The present invention pertains to compds. of the formula (I) (wherein: Q AΒ is O or :NSO2R; R is H or optionally substituted C1-7 alkyl, C3-20 heterocyclyl, or C5-20 aryl; Ar is optionally substituted C5-20 aryl; R1 is H or an oxy substituent such as optionally substituted C1-7 alkyl, C3-20 heterocyclyl, C5-20 heterocyclyl, C5-20 aryl, C1-7 alkylacyl, C3-20 heterocyclyl-acyl, or C5-20 aryl-acyl; the bond marked  $\alpha$  is a single bond or a double bond; the bond marked  $\beta$  is a single bond or a double bond; R3 and R5 are each independently ring substituents; R2 and R6 are each independently ring substituents) and pharmaceutically acceptable salts, esters, amides, solvates, hydrates, and protected forms thereof. The present invention also pertains to pharmaceutical compns. comprising the compds. I, and the use of the compds. I and compns., both in vitro and in vivo, for example, in the treatment of proliferative conditions, (e.g., cancer), mycobacterial infections (e.g., tuberculosis), and/or conditions mediated by thioredoxin/thioredoxin reductase. These compds. I are useful as antiproliferative agents, anticancer agents, antimycobacterial agents, antituberculosis agents, and/or thioredoxin/thioredoxin reductase inhibitors (no data). Thus, to 0.5 g 2-(4-aminophenyl)benzothiazole in 6 mL pyridine was added 0.506 g p-toluenesulfonyl chloride in 4 mL pyridine, heated at reflux for 10 min, cooled, and treated with 10 mL water to 96% N-[(4-benzothiazol-2-yl)phenyl]-4-methylbenzenesulfonamide which (0.1 q) was dissolved in 2 mL MeOH and stirred with BTIB (1.1 15 equivalent) at room temperature for 5 h to give 73% N-[4-methoxy-4-(benzothiazol-2y1)cyclohexa-2,5-dienylidene]-4-methylbenzenesulfonamide (II). 4-(Benzothiazol-2-yl)-4-hydroxy-2,5-cyclohexandien-1-one in vitro showed IC50 of 0.04, 0.38, 0.35, 0.79, and 2.35  $\mu M$  for inhibiting the proliferation of HCT and HT29 human colon carcinoma, human MCF-7 and MDA, 468 breast carcinoma, and A549 human lung adenocarcinoma, resp.

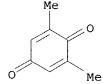
II

IT **527-61-7**, 2,6-Dimethyl-1,4-benzoquinone

RL: RCT (Reactant); RACT (Reactant or reagent) (reactant; preparation of 4-arylquinols and analogs thereof as antiproliferative agents, anticancer agents, antimycobacterial agents, antituberculosis agents, and/or thioredoxin/thioredoxin reductase inhibitors)

RN 527-61-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 6 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2002:556093 HCAPLUS

DOCUMENT NUMBER:

137:105181

TITLE:

Pesticide for control of aquatic pests in

ballast water of ships

INVENTOR(S):

Cutler, Stephen J.; Cutler, Horace G.; Wright, David;

Dawson, Rodger

PATENT ASSIGNEE(S):

USA

SOURCE:

U.S. Pat. Appl. Publ., 11 pp., Cont.-in-part of U.S.

Ser. No. 506,017.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		~ ~ ~ ~ ~ ~ ~ ~		
US-2002098979	A1	20020725	US 2001-3465	20011206
US 63404.68	B1	20020122	US 2000-506017	20000217
US_2002098978	A1	20020725	US 2001-3464	20011206
ŲŠ 65766 <i>7</i> /4	B2	20030610	-	
PRIORITY—APPĹN. INFO.:			US 2000-506017 A	2 20000217
			US 2000-237401P P	20001004

OTHER SOURCE(S):

MARPAT 137:105181

AB The title pesticides are quinones, anthraquinones, naphthalenediones, quinine, warfarin, coumarins, amphotalide, cyclohexadiene-1,4-dione, phenindione, sodium rhodizonate, apirulosin and thymoquinone. The method is particularly effective for treating ballast water of ships or other enclosed vols. of water subject to transport between or among geog. areas to control the relocation of plants, toxic bacteria, and animals contained in the water. The method is especially useful to control zebra mussels in the ballast waters.

106-51-4, 1,4-Benzoquinone, biological studies 319-89-1, Tetrahydroxy-p-benzoquinone 479-22-1, p-Benzoquinone-, 2,5-Dihydroxy-3,6-dinitro 484-89-9, p-Benzoquinone-, 3-hydroxy-2-methoxy-5-methyl 530-55-2 553-97-9 605-94-7, 2,3-DiMethoxy-5-methyl-1,4-Benzoquinone

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(pesticide for control of aquatic pests

in ballast water of ships)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

RN 319-89-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy- (9CI) (CA INDEX NAME)

RN 479-22-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3,6-dinitro- (9CI) (CA INDEX NAME)

$$O_2N$$
  $O_2$   $O_3N$   $O_4$   $O_4$ 

484-89-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)

RN

RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)

RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)

CN

RN 605-94-7 HCAPLUS

2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)

SOURCE:

L20 ANSWER 7 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:859502 HCAPLUS

DOCUMENT NUMBER: 136:270312

TITLE: Photochemical behavior of 4-chloro-2-

methylphenoxyacetic acid Influence of pH and

irradiation wavelength

AUTHOR(S): Zertal, Abdennour; Sehili, Tahar; Boule, Pierre

CORPORATE SOURCE: Departement de Chimie, Laboratoire des Sciences et

Technologie de l'Environnement, Faculte des Sciences, Universite de Constantine, Constantine, 25000, Algeria

Journal of Photochemistry and Photobiology, A:

Chemistry (2001), 146(1-2), 37-48

CODEN: JPPCEJ; ISSN: 1010-6030

Election Calenda C A

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal LANGUAGE: English

The kinetics of phototransformation of 4-chloro-2-methylphenoxyacetic acid (MCPA) is studied under various irradiation conditions. The photocatalytic transformation on TiO2 in aqueous suspension is almost specific and leads to 4-chloro-2-methylphenol (P7) as the main photoproduct. The same product is obtained when MCPA is irradiated on silica in the absence of water. The direct phototransformation is more complex: the reaction is not influenced by oxygen but it depends on the pH of the solution and on the irradiation wavelength. With the anionic form irradiated between 254 and 350 nm, photohydrolysis of C-Cl bond is almost quant. (yield >86%). It leads to the hydroxylated photoproduct P2. With the mol. form the main product P5 results from a photochem. rearrangement of the mol. With both forms, some other photoproducts are also identified and quantified, particularly methylhydroquinone (P1) and P7, 2-methylphenol (P6) is only obtained with the anionic form as a minor product. However, irradiation of solns. in sunlight or with lamps emitting mainly at 365 nm (about 2 and 6% of the light is emitted at 334 and 313 nm, resp.) yields P7 as the main photoproduct. Its formation is self-accelerated. This wavelength effect is attributed to reactions induced by quinonic compds. formed as intermediates since the disappearance of MCPA is more efficient

in presence of quinonic products. P7 is also the major photoproduct when phototransformation is induced by nitrite ions or Fe(III) perchlorate. Besides, it appears from Microtox test that photoproducts formed at wavelength shorter than 350 nm are more toxic to the marine bacterium Vibrio fischeri than the initial compound

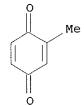
553-97-9P

RL: ADV (Adverse effect, including toxicity); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC

(photoproduct; photochem. of chloromethylphenoxyacetic acid as function of pH and irradiation wavelength and evaluation of photoproducts toxicity to marine bacterium Vibrio fischeri)

553-97-9 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME) CN



REFERENCE COUNT: THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS 31 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2004 ACS on STN L20 ANSWER 8 OF 44

2001:626671 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 136:8952

Photosynthetic bioelectrochemical cell utilizing TITLE:

cyanobacteria and water-generating oxidase

Tsujimura, S.; Wadano, A.; Kano, K.; Ikeda, T. AUTHOR(S):

Graduate School of Agriculture, Division of Applied CORPORATE SOURCE:

Life Sciences, Kyoto University, Sakyo, Kyoto,

606-8502, Japan

Enzyme and Microbial Technology (2001), 29(4-5), SOURCE:

225-231

CODEN: EMTED2; ISSN: 0141-0229

Elsevier Science Ireland Ltd. PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

A novel photosynthetic bioelectrochem. cell that utilizes biocatalysts in both anode and cathode compartments was constructed for the first time. in the anodic half-cell, some parts of the electrons produced by the oxidation of water in the photosystem of cyanobacteria are transferred to the carbon felt anode through quinonoid electron transfer mediators. electron is passed to dioxygen to regenerate water in the cathodic half-cell reaction with an aid of bilirubin oxidase reaction via a mediator. The maximum elec. power was about 0.3-0.4 W m-2 for the projective electrode surface area at an apparent efficiency of the light energy conversion of 2-2.5%. The factors governing the cell output are discussed on the basis of the potential-current curves of each half-cell. IT

**527-61-7**, 2,6-Dimethyl-1,4-benzoquinone

RL: DEV (Device component use); USES (Uses) (photosynthetic bioelectrochem. cell utilizing cyanobacteria

and water-generating oxidase)

527-61-7 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl- (9CI) (CA INDEX NAME) CN

REFERENCE COUNT:

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS 35 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 9 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2001:618136 HCAPLUS

DOCUMENT NUMBER:

135:191666

TITLE:

Biocidal compds. for controlling populations of

aquatic pest organisms containing quinones,

anthraquinones, and naphthalenediones

INVENTOR(S):

Cutler, Horace; Cutler, Stephen; Wright, David;

Dawson, Rodger

PATENT ASSIGNEE(S):

Garnett, Inc., USA

SOURCE:

PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.																
								WO 2001-US5117								216	
WO	2001	0609	71		A3		2001	1213									
	W:	ΑE,	AG,	AL,	AM,	AT,	AT,	AU,	ΑZ,	BA	, BB	, BG,	BR,	BY,	BZ,	CA,	CH,
		CN,	CR,	CU,	CZ,	CZ	DE,	DE,	DK,	DK	, DM	, DZ,	EE,	EE,	ES,	FI,	FΙ,
		GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL	, IN	, IS,	JP,	KE,	KG,	ΚP,	KR,
		KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA	, MD	, MG,	MK,	MN,	MW,	MX,	MZ,
		NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG	, si	, sk,	SK,	SL,	TJ,	TM,	TR,
		TT,	TZ,	UA,	UG,	US,	UZ,	VN,	ΥU,	ZA	, ZW	, AM,	ΑZ,	BY,	KG,	KZ,	MD,
		RU,	TJ,	TM													
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ	, TZ	, UG,	ZW,	ΑT,	BE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	ΙΊ	LU,	, MC,	NL,	PT,	SE,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML	, MR	, NE,	SN,	TD,	TG		
US	6340											-5060				0000	217
CA	2406	968			AA		2001	0823		CA	2001	-2406	968		2	0010	216
	2001																
EP	1261	254			A2		2002	1204		EΡ	2001	-9127	84		2	0010	216
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		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL	, TR						
JР	2003	5238	21		Т2		2003	0812		JP	2001	-5603	43		2	0010	216
EE	2002	0045	5		Α		2003	1215		EE	2002	-455			2	0010	216
US	2002	0989	78		A1		2002	0725		US	2001	-3464			2	0011	206
US	6576	674			B2		2003	0610									
	2002						2002	1007		NO	2002	-3912			2	0020	816
	1071						2003			BG	2002	-1071	08		2	0020	916
PRIORIT	Y APP	LN.	INFO									-5060				0000	217
										US	2000	-2374	01P		P 2	0001	004
												-US51			W 2	0010	216
OTHER S	OURCE	(S):			MAR	PAT	135:	1916	66								

OTHER SOURCE(S):

GI

III

 $R^4$ 

Biocidal compds. for controlling populations of aquatic pest AΒ microorganisms, plants or animals are selected from the group consisting of naphthalenediones I (R1 = H, OH, Me; R2 = H, Me, sodium bisulfate, C1, acetonyl, 3-methyl-2-butenyl, 2-oxypropyl;R3 = H, Me, Cl, methoxy, or 3-methyl-2-butenyl; R4 = H, methoxy; R5 = H, OH, Me; R6 = H, OH), quinones II (R1 = H, Me, OH, methoxy; R2 = H, OH, Me, methoxy, NO2; R3 = H, OH, Me, methoxy; R4 = H, Me, methoxy, OH, NO2), anthraquinones III (R1 = H, OH, C1;R2 = H, Me, C1, OH, carbonyl, carboxyl; R3 = H, Me; R4 = H; R5 = H, OH; R6, R7 = H; R8 = H, OH), quinine, warfarin, coumarins, amphotalide, cyclohexadiene-1,4-dione, phenidione, pirdone, sodium rhodizonate, apirulosin, thymoquinone,. The compds. are used to control population of target pest microorganisms is selected from the group consisting of viruses, protists, holoplanktonic organisms, and meroplanktonic organisms, demersal organisms, benthic organisms, detached or floating biota, bacteria, encysted bacteria, protozoans, algae, pyrrophyta, cryptophyta, chrysophyta, porifera, platyhelminthes, pseudocoelomates, annelid worms, zebra mussels, bivalves, larval forms of copepods, ostracods, mysids, gammarids, larval forms of decapods, and larval teleost fish. The method is particularly effective for treating ballast water of ships or other enclosed vols. of water subject to transport between or among geog. areas to control the relocation of plants, bacteria, and animals contained in the water.

106-51-4, Cyclohexadiene-1,4-dione, biological studies

319-89-1, Tetrahydroxy-p-benzoquinone 479-22-1

484-89-9, 3-Hydroxy-2-methoxy-5-methyl-p-benzoquinone

530-55-2 553-97-9 605-94-7

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(biocidal compds. for controlling populations of aquatic pest organisms containing)

RN 106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

IT

CN

Ŕ5

RN 319-89-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy- (9CI) (CA INDEX NAME)

RN 479-22-1 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3,6-dinitro- (9CI) (CA INDEX NAME)

RN 484-89-9 HCAPLUS

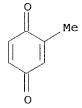
CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)

RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)

RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



605-94-7 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX CN NAME)

L20 ANSWER 10 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:109589 HCAPLUS

DOCUMENT NUMBER:

134:359368

TITLE:

Electrochemical investigation of cyanobacteria

Synechococcus sp. PCC7942-catalyzed photoreduction of exogenous quinones and photoelectrochemical oxidation

of water

AUTHOR(S):

Torimura, M.; Miki, A.; Wadano, A.; Kano, K.; Ikeda,

CORPORATE SOURCE:

Division of Applied Life Sciences, Graduate School of

Agriculture, Kyoto University, Kyoto, Sakyo, 606-8502,

Japan

SOURCE:

Journal of Electroanalytical Chemistry (2001),

496(1-2), 21-28

CODEN: JECHES; ISSN: 0368-1874

PUBLISHER:

Elsevier Science S.A.

LANGUAGE:

DOCUMENT TYPE: Journal English

The electron transfer from the photosynthetic system in cyanobacteria, AB Synechococcus sp. PPC7942 to exogenous electron acceptors was examined using several electrochem. techniques. 1,4-Benzoquinone (BQ) and 2,6-dimethyl-1,4-benzoquinone (DMBQ) were found to function as good exogenous electron acceptors for the photosystem. Kinetic anal. with rotating disk amperometry revealed that the photoredn. of these quinones proceeds in Michaelis-Menten type kinetics for the concentration of the quinones and the light intensity. The electron transfer rate of the BQ reduction was as high as 68% compared with that of the photosynthetic oxygen evolution. Synechococcus sp. cell-entrapped and DMBQ-embedded carbon paste electrodes provided steady-state current ascribed to the photoelectrochem. oxidation of water. Although several inhibitors against the photosynthetic system suppressed the photoelectrochem. response, phenylmercury acetate, which inhibits ferredoxin and ferredoxin-NADP oxidoreductase, was found to enhance the photocurrent. Some electrochem. aspects of this system are discussed.

TT 106-51-4, 1,4-Benzoquinone, reactions 527-61-7,

2,6-Dimethyl-1,4-benzoquinone

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC

(Process); RACT (Reactant or reagent)

(electrochem. investigation of **cyanobacteria** Synechococcus sp. PCC7942 catalyzed photoredn. of exogenous quinones and photoelectrochem. oxidation of **water**)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

CN

RN 527-61-7 HCAPLUS

2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl- (9CI) (CA INDEX NAME)

Me O Me

REFERENCE COUNT:

51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 11 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:773826 HCAPLUS

DOCUMENT NUMBER: 134:96495

TITLE: Sediment mutagenicity testing: Development of

substance specific bacterial strains for the detection of mutagenic aromatic nitrogen compounds and oxidative

mutagens

AUTHOR(S): Vahl, H. H.; Karbe, L.; Prieto-Alamo, M. J.; Pueyo,

C.; Westendorf, J.

CORPORATE SOURCE: Department of Toxicology, Medical School, University

of Hamburg, Hamburg, D-22527, Germany

SOURCE: Aquatic Ecosystem Health & Management (2000), 3(3),

360-378

CODEN: AEHMF4; ISSN: 1463-4988

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

The arabinose resistance forward mutation assay was chosen for the development of bacterial strains in order to get specific mutagenic responses. Special strains of Salmonella typhimurium were constructed which show an elevated expression of nitroreductase and O-acetyltransferase. They were shown to be highly sensitive to mutagenic nitro-compds. (e.g. 1-nitropyrene and 1,8-dinitropyrene) and, after metabolic activation by rat liver S9-mix, also to mutagenic amino-compds. (2-aminoanthracene). Furthermore, strains of Escherichia coli with reduced expression of antioxidative enzymes (catalase and superoxide dismutase) were constructed. However, they were only moderately sensitive to oxidative mutagens such as quinones, nitrogen compds., and the herbicide paraquat, because, in contrast to the Salmonella strains used, they build up a complete gram-neg. cell wall. For this reason, the Escherichia strains were further genetically altered in order to make their cell wall penetrable to lipophilic compds. This alteration increased the sensitivity to more lipophilic compds. The strains were

more sensitive to 1-nitropyrene by a factor of more than 10 and to 1,8-dinitropyrene by a factor of more than 100. In order to validate the arabinose resistance test with the newly constructed strains, sediments of the whole German part of the Elbe River were examined Overall mutagenicity (standard strains) as well as enhanced effects with the special strains were observed in sediment samples of the river. Mutagenic hot spots reflect direct industrial influences as well as hydrol. situations, which has led to concentration of the organic content of suspended matter, loaded with industrial or rural contamination. Generally, high mutagenic effects were observed where chemical analyses showed a high degree of contamination.

106-51-4, Quinone, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (sediment mutagenicity testing and development of substance specific bacterial strains for the detection of mutagenic aromatic nitrogen compds. and oxidative mutagens).

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

IT

CN

REFERENCE COUNT:

THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS 33 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 12 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2000:213642 HCAPLUS 132:212299

DOCUMENT NUMBER:

Quinone profiles in lake sediments: implications for

microbial diversity and community structures

AUTHOR(S):

TITLE:

SOURCE:

Hiraishi, Akira; Kato, Kenji

CORPORATE SOURCE:

Department of Ecological Engineering, Toyohashi

University of Technology, Toyohashi, 441-8580, Japan Journal of General and Applied Microbiology (1999),

45(5), 221-227

CODEN: JGAMA9; ISSN: 0022-1260

PUBLISHER:

Microbiology Research Foundation

DOCUMENT TYPE:

Journal

LANGUAGE: English

Microbial quinone compns. of sediment mud samples from 5 lakes in Japan were studied by spectro-chromatog, and mass spectrometry. Total quinone content of these samples was 1.97-18.0 nmol/q dry weight sediment, of which a combined fraction of ubiquinones and menaquinones accounted for 42-74%. The remaining fraction (26-58%) consisted of the photosynthetic quinones, plastoquinones and phylloquinone. Sediment samples produced PQ-9 or Q-8 as the most abundant quinone type regardless of their geog. location and depth. Results indicated that oxygenic phototrophic microorganisms and Q-8-containing proteobacteria constituted major parts of microbial populations in lake sediment. In surface water of the same sampling sites, plastoquinones and phylloquinone occurred in much higher proportions. These findings suggested the abundance of oxygenic phototrophs in sediment muds resulted from their constant movement or sedimentation from the surface water. Numerical analyses of quinone profiles showed that sediment microbial communities were diverse and different in different lakes, but similar to each other in the diversity of bio-energetic modes. Three physiol. groups of microbes exhibiting ubiquinone-mediated aerobic respiration, oxygenic photosynthesis, and menaquinone-associated respiration, were suggested to inhabit the lake sediment in balance. IT

106-51-4, Quinone, biological studies

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); OCU (Occurrence, unclassified); BIOL (Biological study); OCCU (Occurrence) (bacterial; lake sediment quinone profiles and their implication for microbial diversity and community structures)

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

CN

REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

L20 ANSWER 13 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

17

1999:385535 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 131:155862

Investigation on the detergent role in the function of TITLE:

secondary quinone in bacterial reaction centers

Agostiano, Angela; Milano, Francesco; Trotta, Massimo

AUTHOR(S): Dipartimento di Chimica, Universita di Bari, Bari, CORPORATE SOURCE:

I-70126, Italy

European Journal of Biochemistry (1999), 262(2), SOURCE:

358-364

CODEN: EJBCAI; ISSN: 0014-2956

PUBLISHER: Blackwell Science Ltd.

DOCUMENT TYPE: Journal English LANGUAGE:

In this paper are reported studies on the detergent role in isolated reaction centers (RC) from Rhodobacter sphaeroides, over a large range of lauryldimethylamino-N-oxide (LDAO) concns., in influencing the thermodn. of the quinone exchange reaction as well as the protein aggregation. The occurrence of the quinone exchange reaction between the QB-binding site (where QB is the second quinone mol. of two in the RC) and the ubiquinone O dissolved in the different environments (water, LDAO micelles and detergent phase of the protein-detergent complex) has also been analyzed. Measurements carried out in QB-depleted RC to which exogenous quinone has been added show that the relative amplitudes of the slow and fast phase of the recombination reaction depend on this parameter. The overall amount of the restored QB-functionality is affected by the concentration of the LDAO in solution Interpolation of the titration curves with a quadratic function obtained by simple considerations allowed the binding constant of UQO to the QB-binding site to be calculated From the fitting procedure, the distribution of the quinone in the different environments present in solution was evaluated, indicating that the exchange reaction can take place only between the QB-site and the detergent phase. The dependence of the quinone pool size upon the volume of the phase in which the interacting quinone is solubilized is also discussed. The increasing difficulty in saturating the QB-pocket above the LDAO critical micellar concentration is finally related to the association of protein-detergent complexes to form large protein clusters.

605-94-7, Ubiquinone 0 TT

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(detergent role in the function of secondary quinone in

bacterial reaction centers)

605-94-7 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX CN NAME)

REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS 36

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 14 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:573580 HCAPLUS

DOCUMENT NUMBER:

125:214499

TITLE:

Benzo[a]pyrene metabolism and xenobiotic-stimulated

reactive oxygen species generation by subcellular

fraction of larvae of turbot (Scophthalmus maximus L.) Peters, L. D.; O'Hara, S. C. M.; Livingstone, D. R.

AUTHOR(S): CORPORATE SOURCE: NERC Plymouth Marine Laboratory, Devon, PL1 2PB, UK SOURCE: Comparative Biochemistry and Physiology, C:

Pharmacology, Toxicology and Endocrinology (1996),

114C(3), 221-227

CODEN: CBPCEE; ISSN: 0742-8413

PUBLISHER: DOCUMENT TYPE:

Elsevier Journal LANGUAGE: English

NADPH-dependent 3H-benzo[a]pyrene (BaP) metabolism and basal and xenobiotic-stimulated NAD(P)H-dependent reactive oxygen species (ROS) production were investigated in 11,600 g supernatants of 4-day-old (yolk sac) larvae of turbot (Scophthalmus maximus L.). BaP metabolites were resolved by HPLC and detected radiometrically. ROS were quantified by the iron-EDTA mediated production of hydroxyl radical (.OH) that was detected by its oxidation of 2-keto-4-methiobutyric acid (KMBA) to yield ethylene. BaP metabolism produced phenols, dihydrodiols and diones (quinones) (resp., 54, 32, and 14% of free metabolites) and putative protein adducts. Metabolites identified by retention time included the 7,8-dihydrodiol, the 1,6-, 3,6- and 6,12-diones and the 3- and 9-phenols. Pre-exposure of turbot larvae to 5 ppb BaP for 24 h caused an approx. 2-fold increase in both BaP metabolism and 7-ethoxyresorufin O-deethylase activity, indicative of the induction of cytochrome P 4501A and its involvement in BaP metabolism Basal KMBA oxidation rates were similar for NADH and NADPH. Inhibition studies indicate that OH was formed via the production of superoxide anion radical and hydrogen peroxide. Basal ROS production was stimulated up to 3-fold by a range of redox cycling aromatic hydrocarbon quinones and indicated to be stimulated by other xenobiotics, including nitroaroms. The results indicate biotransformation and ROS production as potential mechanisms of toxicity in larval fish.

IT 106-51-4, 1,4-Benzoquinone, biological studies 527-17-3, Duroquinone

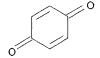
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(benzopyrene metabolism and xenobiotic-stimulated reactive oxygen species generation by subcellular fraction of larvae of turbot)

RN106-51-4 HCAPLUS

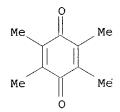
CN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN527-17-3 HCAPLUS

2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME) CN



HCAPLUS COPYRIGHT 2004 ACS on STN L20 ANSWER 15 OF 44

ACCESSION NUMBER:

1992:101103 HCAPLUS

DOCUMENT NUMBER:

116:101103

TITLE:

SOURCE:

Reduction of ethylenethiourea content in alkylenebisdithiocarbamate fungicides, using

hydroxymethane sulfinate

INVENTOR(S):

Diepenhorst, Pieter Carel; Kool, Pieter; Nouws,

Jacobus Adrianus Maria

PATENT ASSIGNEE(S):

Atochem Agri S. A., Fr. Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT	NO.			KIND	)	DATE		AP:	APPLICATION NO.					Έ
	EP 4606	12			<b>A</b> 1		1991	1211	EP	1991-	1091	26		199	10604
	EP 4606	12			B1		1995	0510							
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, G	R, IT,	LI,	LU,	NL,	SE	
	US 5100	915			Α		1992	0331	US	1990-	5339	67		199	00606
	AU 9178	045			<b>A</b> 1		1991	1212	AU	1991-	7804	5		199	10530
	AU 6402	33			B2		1993	0819							
	JP 0423	5957			A2		1992	0825	JP	1991-	1594	98		199	10604
	JP 2872	448			B2		1999	0317				X			
	AT 1222	06			E		1995	0515	AT	1991-	1091	26		199	10604
	ES 2071	862			Т3		1995	0701	ES	1991-	1091	26		199	10604
	BR 9102	335			Α		1992	0107	BR	1991-	2335			199	10605
PRIOR	ITY APP	LN.	INFO	. :					US	1990-	5339	67	I	199	00606
AB .	A metho	d is	pro	vided	l for	st	abil.	izing	g alky	lenebi	sdit	hioca	arbam	nates,	such

A method is provided for stabilizing alkylenebisdithiocarbamates, such as 1,2-ethylenebisdithiocarbamates (EBDC), by mixing the EBDC in the presence of water with hydroxymethanesulfinate (HMS) which degrades to HCHO to reduce the content of ethylenethiourea (ETU) in the EBDC. The HMS and sulfite byproduct from the HCHO formation also act as reducing agents to inhibit further ETU formation by oxidative decomposition of EBDC. The HMS is preferably added at 0.1-5% by weight, based upon the EBDC, and the aqueous reaction mixture is then preferably dried under vacuum. Copolymn. agents, such as hydroquinone or melamine, may also be added to further reduce and inhibit ETU formation. Mancozeb (4 g) was treated with 50 mg HMS Na salt

and 10 mL water, followed by drying. After 45 days, the ETU content was decreased to 0.01% from the original 0.05%. 106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies

RL: BIOL (Biological study)

(alkylenebisdithiocarbamate fungicides stabilization by hydroxymethanesulfinate and, decrease in ethylenethiourea content in relation to)

106-51-4 HCAPLUS RN

CN2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



IT

HCAPLUS COPYRIGHT 2004 ACS on STN L20 ANSWER 16 OF 44

ACCESSION NUMBER: 1991:625722 HCAPLUS

115:225722 DOCUMENT NUMBER:

Quantitative structure-activity relationships for TITLE:

chemical toxicity to environmental bacteria

AUTHOR (S): Blum, Diane J. W.; Speece, R. E.

Bala Cynwyd, PA, 19004, USA CORPORATE SOURCE:

Ecotoxicology and Environmental Safety (1991), 22(2), SOURCE:

198-224

CODEN: EESADV; ISSN: 0147-6513

DOCUMENT TYPE: Journal LANGUAGE: English'

OSARs were developed for nonreactive chemical toxicity to each of four groups of bacteria of importance in environmental engineering: aerobic heterotrophs, methanogens, Nitrosomonas, and Microtox. The QSARs were based on chems. covering a range of structures and including important environmental pollutants (i.e., chlorinated and other substituted benzenes, phenols, and aliphatic hydrocarbons). QSARs were developed for each chemical class and for combinations of chemical classes. Three QSAR methods (groups of chemical describing parameters) were evaluated for their accuracy and ease of use: log P, linear solvation energy relationships (LSER), and mol. connectivity. Successful QSARs were found for each group of bacteria and by each method, with correlation coeffs. (adjusted r2) between 0.79 and 0.95. LSER QSARs incorporated the wildest range of chems. with the greatest accuracy. Log P and mol. connectivity QSARs are easier to use because their parameters are readily available. Outliers from the QSARs likely due to reactive toxicity included acryls, low pKA compds., and aldehydes. Nitro compds. and chlorinated aliphatic hydrocarbons and alcs. showed enhanced toxicity to the methanogens only. Chems. with low IC50 concns. (log IC50  $\mu mol/L$  < 1.5) were often outliers for Nitrosomonas. QSARs were validated statistically and with literature data. A suggested method is provided for use of the QSARs.

106-51-4, 1,4-Benzoquinone, biological studies IT

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to environmental bacteria, mol. structure effect on)

RN 106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN



L20 ANSWER 17 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1988:147323 HCAPLUS

DOCUMENT NUMBER:

108:147323

TITLE:

Characterization of protonmotive force generation in liposomes reconstituted from phosphatidylethanolamine,

reaction centers with light-harvesting complexes

isolated from Rhodopseudomonas palustris

AUTHOR(S):

Molenaar, Douwe; Crielaard, Wim; Hellingwerf, Klaas J.

Dep. Microbiol., Univ. Groningen, Haren, 9751 NN, CORPORATE SOURCE:

Neth.

SOURCE:

Biochemistry (1988), 27(6), 2014-23

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE:

Journal LANGUAGE: English

Reaction center complexes were isolated from R. palustris with either one ΔR or both of the light-harvesting complexes attached. Both complexes were incorporated into liposomes made of phospholipids purified from Escherichia coli. Light-driven cyclic electron transport could be restored in these proteoliposomes upon the addition of the redox mediators cytochrome c and a water-soluble ubiquinone. During cyclic electron transport in this artificial system, protons are extruded electrogenically from the liposomes, and this leads to the generation of a protonmotive force (PMF). The optimal conditions for PMF generation were pH 8, a reaction center/lipid ratio of 1.4 nmol/mg, and cytochrome c and ubiquinone 0 concns. of 10 and 400 μM, resp. The maximum membrane potential generated under these conditions was -180 mV. From titration

No

evidence was obtained for a contribution of light-harvesting complex II to PMF generation; i.e., these complexes are functionally uncoupled from the reaction centers. Neither was an electrochromic band shift of the carotenoids, present in these complexes, measurable upon illumination. A kinetic model representing the artificial redox chain cytochrome c/reaction center/ubiquinone 0 is presented. For this model, data have been used from fast kinetic studies on reaction centers from Rhodobacter sphaeroides. The model explains the observed discrepancy between the dissociation constant (Kd) of reaction centers for cytochrome c and the Michaelis constant (Km for the rate of cytochrome c oxidation The model also explains the light dependency of this Km.

studies with a protonophore, it was found that the intrinsic maximum capacity

of the reaction centers in PMF generation (the electromotive force) equals -210 mV.

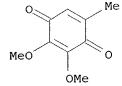
605-94-7, Ubiquinone 0 IT

RL: BIOL (Biological study)

(reconstituted liposomes containing bacterial reaction centers and, protonmotive force generation in relation to)

605-94-7 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX CN



L20 ANSWER 18 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:105130 HCAPLUS

DOCUMENT NUMBER: 106:105130

TITLE: Coal extraction by aprotic dipolar solvents

AUTHOR(S): Sears, J. T.

CORPORATE SOURCE: Montana State Univ., Bozeman, MT, USA

SOURCE: Report (1985), DOE/PC/50787-T6; Order No. DE86005354,

175 pp. Avail.: NTIS

From: Energy Res. Abstr. 1986, 11(8), Abstr. No. 15507

DOCUMENT TYPE: Report LANGUAGE: English

The extraction of coal at low temps. by a class of solvents with a generic structure, including Me2NCOHME2 [632-22-4] and (Me2N)3PO [680-31-9], was used to examine the nature of the extracted coal chems. The class of solvents with similar action, however, can be classified as aprotic, base solvents or, somewhat more broadly, specific solvents. The action of the solvents was then examined to postulate a mechanism of attack. Exptl. work conducted to explain the specific solvent attack included (1) pure solvent extraction, (2) extraction with mixts. with otherwise inert solvents and inhibitors, and (3) extraction with simultaneous catalytic enhancement attempts, including water-gas shift conversion. Thus, NMR and gas chromatog./mass spectroscopy of extract mols. and extraction with high-pressure CO in Me2HCONMe2 (containing 2% H2O) was performed. The effects of solvent additives, such as cumene [98-82-8] and quinone [106-51-4], in large amts. of inert solvents, such as Tetralin [119-64-2], liminone [106908-29-6], or CS2, on extraction were also determined

L20 ANSWER 19 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:439218 HCAPLUS

DOCUMENT NUMBER: 105:39218

TITLE: Coincident plasmids and antimicrobial resistance in

marine bacteria isolated from polluted and unpolluted

Atlantic Ocean samples

AUTHOR(S): Baya, A. M.; Brayton, P. R.; Brown, V. L.; Grimes, D.

J.; Russek-Cohen, E.; Colwell, R. R.

CORPORATE SOURCE: Dep. Microbiol., Univ. Maryland, College Park, MD,

20742, USA

SOURCE: Applied and Environmental Microbiology (1986), 51(6),

1285-92

CODEN: AEMIDF; ISSN: 0099-2240

DOCUMENT TYPE: Journal LANGUAGE: English

AB Sewage effluent and outfall confluence samples were collected at the Barceloneta Regional Treatment Plant in Barceloneta, Puerto Rico; outfall confluence samples at Ocean City, Md., were also collected. Samples from uncontaminated open ocean areas served as clean-water controls. Bacteria were enriched in marine broth 2216 amended with 1 μg of one of a set of chemical selected for study per mL: nitrobenzene, di-Bu phthalate, m-cresol, o-cresol, 4-nitroaniline, bis(tributyltin) oxide, and quinone. Min. inhibitory concns. of the chemical were determined individually for all isolates. Bacterial isolates were evaluated for resistance to 9 different antibiotics and for the presence of plasmid DNA. Treated sewage contained

large nos. of bacteria simultaneously possessing antibiotic resistance, chemical resistance, and multiple bands of plasmid DNA. Bacteria resistant to penicillin, erythromycin, nalidixic acid, ampicillin, m-cresol, quinone, and bis(tributyltin) oxide were detected in nearly all samples, but only sewage outfall confluence samples yielded bacterial isolates that were resistant to streptomycin. Bacteria resistant to a combination of antibiotics, including kanamycin, chloramphenicol, gentamicin, and tetracycline, were isolated only from sewage effluent samples. Thus, bacterial isolates derived from toxic chemical wastes more frequently contain plasmid DNA and demonstrate antimicrobial resistance than do bacterial isolates from domestic sewage-impacted waters or from uncontaminated open ocean sites.

106-51-4, biological studies RL: BIOL (Biological study) IT

(plasmid-mediated resistance to, in marine bacteria,

water pollution in relation to)

RN 106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

CN

HCAPLUS COPYRIGHT 2004 ACS on STN L20 ANSWER 20 OF 44

ACCESSION NUMBER: 1985:499810 HCAPLUS

DOCUMENT NUMBER: 103:99810

TITLE: Combined action of heavy metals and phenols on

aquatic organisms

Gil, T. A.; Saksonov, M. N.; Stom, D. I. AUTHOR(S):

NII Biol., Irkutsk, USSR CORPORATE SOURCE:

Vodnye Resursy (1985), (3), 118-21 SOURCE:

CODEN: VDRSBK; ISSN: 0321-0596

DOCUMENT TYPE: Journal

Russian LANGUAGE:

In suspensions of Beneckea harveyi exposed to mixts. of HgCl2 with p-benzoquinone (I) [106-51-4], resorcine [108-46-3] or hydroquinone [123-31-9] (5 min at 21°, pH 6.0), the fluorescence of the bacteria decreased in correlation with the concns. of both components. The decreases were additive, synergic, or antagonistic, depending on the concns. of the components. Thus, for the determination of maximum permissible concns. of water pollutants, it is not sufficient to consider only the concns. of each of the pollutants alone.

L20 ANSWER 21 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:424507 HCAPLUS

DOCUMENT NUMBER: 103:24507

TITLE: Hexanitrostilbene

INVENTOR(S): Duffin, Henry Charles; Golding, Peter;

Jaweera-Bandara, Asoka Manitha

PATENT ASSIGNEE(S):

United Kingdom Secretary for Defence, UK

Eur. Pat. Appl., 25 pp. SOURCE:

CODEN: EPXXDW

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 132990	A2	19850213	EP 1984-304895	19840718
EP 132990	ДЗ	19850313		
EP 132990	B1	19870902		
R: DE, FR, GB,	SE		•	
GB 2144736	A1	19850313	GB 1983-19850	19830722
US 4626606	Α	19861202	US 1984-632294	19840719
PRIORITY APPLN. INFO.:			GB 1983-19850 A	19830722
AB HNS [20062-22-0] i	s synth	esized by o	xidizing TNT [118-96-7]	or

1,2-dipicrylethane (I) [5180-53-0] with free O, H2O2, or a benzoquinone in a medium containing an aprotic solvent, a protic solvent, and a basic alkali metal carboxylate. Thus, 0.64 g NaOBz [532-32-1] in 25 mL DMSO [67-68-5] was slowly added at 800 rpm to a solution of 1.9 g I in 25 mL DMSO at 25°. Dry air was pumped through the blue solution at .apprx.2 L/s until the color changed to red-brown (after .apprx.30 min), and the reaction was quenched by pouring into 100 mL water acidified with 1 mL concentrated HCl. The precipitate was isolated after standing for 10 min

and

dried at 60°. The yield of crude product was 0.96 g (96 mol%). Washing with MeOH and acetone to remove byproducts and DMSO gave 0.64 q (64 mol%) pure HNS. Solvent stripping of the acetone filtrate and drying gave 0.17 g (17 mol%) unreacted I. Conversion of I to other water -soluble byproducts was 0.15 g (15 mol%).

106-51-4, uses and miscellaneous TT

RL: USES (Uses)

(oxidizing agents, in HNS synthesis from dipicrylethane and TNT in presence of aprotic and protic solvents and alkali metal carboxylate catalysts)

106-51-4 HCAPLUS RN

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L20 ANSWER 22 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1985:137411 HCAPLUS

DOCUMENT NUMBER:

102:137411

TITLE:

Removal of quinones from an aqueous environment by

phenols and the effect of their mixing on the luminescence of the bacteria Beneckea harveyi

Gil, T. A.; Nechaeva, V. I.; Balayan, A. E.; Shakhova, AUTHOR(S):

G. V.; Stom, D. I.; Koryakovtsev, A. A.

CORPORATE SOURCE:

Irk. Gos. Univ., Irkutsk, USSR

SOURCE:

Biologicheskie Nauki (Moscow) (1985), (1), 58-62

CODEN: BINKBT; ISSN: 0470-4606

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

The addns. of monobasic phenols to water containing p-benzoquinone

(I) [106-51-4] decreased I concentration as determined by the potentiometric titration, polarog., and bioassay (luminescence of Benecka harvey bacteria and life span of Daphnia pulex). Thus, the addition of 10-2 M solution resorcinol [108-46-3] to an equal volume of 10-3 M I solution decreased I concentration by 78.5% in 30 min. This effect was due to I interactions with phenols leading to polyphenols of reduced bioactivity.

L20 ANSWER 23 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:73749 HCAPLUS

DOCUMENT NUMBER: 102:73749

TITLE: Glutathione S-transferase in aquatic

macroinvertebrates and its interaction with different

organic micropollutants

AUTHOR(S): Dierickx, Paul J.

CORPORATE SOURCE: Inst. Hyg. Epidemiol., Brussels, B-1050, Belg.

SOURCE: Science of the Total Environment (1984), 40, 93-102

CODEN: STENDL; ISSN: 0048-9697

DOCUMENT TYPE: Journal LANGUAGE: English

The presence of GSH S-transferase (GST) [50812-37-8] in aquatic AB macroinvertebrates and its possible significance as a detoxification mechanism of organic micropollutants in the aquatic environment was investigated. GST was found in 20 macroinvertebrates (in adults as well as in larvae) and in insects as well as in other animal groups. The GST activities were relatively high, ranging from 10 to 600% of the activity found in rat liver. The interaction of quinones, o-chloranil [2435-53-2], and chlorophenoxyalkyl acids with the GST activity, in exts. from 3 different macroinvertebrates, revealed an inhibition which was quite similar to that previously found for rat liver GST. In Tubifex tubifex exts., at least 3 different GST isoenzymes could be demonstrated. These partially purified isoenzymes were used for the kinetic anal. of GST inhibition by 2,4-dichlorophenoxyalkyl acid and 1,4-benzoquinone 106-51-4], using Lineweaver-Burk plots. The same kinetic patterns were observed as for rat liver GST. Interactions of the compds. investigated with aquatic macroinvertebrate and with rat liver GST were in very good agreement. Thus, macroinvertebrate GST may play a key role in the detoxification of organic micropollutants in the aquatic environment.

L20 ANSWER 24 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:60757 HCAPLUS

DOCUMENT NUMBER: 102:60757

TITLE: Oxygen supply to immobilized cells. 4. Use of

p-benzoquinone as an oxygen substitute

AUTHOR(S): Adlercreutz, Patrick; Mattiasson, Bo

CORPORATE SOURCE: Chem. Cent., Univ. Lund, Lund, S-220 07, Swed.

SOURCE: Applied Microbiology and Biotechnology (1984), 20(5),

296-302

CODEN: AMBIDG; ISSN: 0175-7598

DOCUMENT TYPE: Journal LANGUAGE: English

O2 supply is a critical point in tech. processes when aerobic cells are used in immobilized prepns. In this study, p-benzoquinone [106-51-4] is used as a substituent for O2 in the oxidation of glycerol [56-81-5] to dihydroxyacetone [96-26-4] by immobilized Gluconobacter oxydans cells. The reaction rate was much higher when p-benzoquinone was used compared to when O2 was used. In an experiment with free cells, p-benzoquinone gave a rate >4-fold that of O2, and with immobilized cells, the difference was even greater. p-Benzoquinone is more effective than O2, because it gives a higher maximal reaction rate (the reason for this fact is discussed) and because it is more soluble in water than O2. The operational stability of the process is comparatively good. In 1 experiment,

the productivity decreased from 60 to 10 mmol/h-q over an 8-day period when p-benzoquinone was used. When O2 was used in a similar experiment, the productivity decreased from 14 to 6 mmol/h-g. The byproduct formed from p-benzoquinone, hydroquinone, can be oxidized to p-benzoquinone, which can be reused. Seven successive regenerations of p-benzoquinone were performed without any loss of efficiency.

106-51-4, biological studies RL: BIOL (Biological study)

> (as oxygen substitute, in glycerol oxidation to dihydroxyacetone by immobilized Gluconobacter oxydans)

106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



IT

RN

CN

L20 ANSWER 25 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1984:494445 HCAPLUS

DOCUMENT NUMBER:

TITLE:

Photoproduction of hydrogen using plant and microbial

membrane systems. Final subcontract report

AUTHOR(S):

LANGUAGE:

Olson, J. M.

CORPORATE SOURCE:

Brookhaven Natl. Lab., Upton, NY, USA

SOURCE:

Report (1983), SERI/STR-231-1874; Order No.

DE84000062, 35 pp. Avail.: NTIS

From: Energy Res. Abstr. 1984, 9(9), Abstr. No. 16095

DOCUMENT TYPE:

Report English

A solar H generator was assembled from unit-membrane vesicles from green photosynthetic bacteria. The vesicles contain light-harvesting bacteriochlorophyll a [17499-98-8], photochem. reaction centers, and various electron carriers that deliver electrons from ascorbic acid [50-81-7] to exogenous ferredoxin and hydrogenase [9027-05-8]. H is formed with an overall quantum requirement of .apprx.10 photons/electron transferred. Of 21 polypeptides found in the vesicle membranes 5 (25.0, 25.5, 38.5, 69, and 93 kD) have the possibility of a specific association with the reaction center. Another type of photosynthetic membrane from a thermophilic cyanobacterium contains both photosystem I and photosystem II reaction centers. Photosystem II particles prepared with lauryl dimethylamine oxide [1643-20-5] evolve O from H2O and deliver electrons to a weak reductant, dimethylbenzoquinone [30998-92-6 ], with an overall quantum requirement of .apprx.5 photons/electron. If vesicles from green bacteria can be coupled to membranes or photosystem II particles from cyanobacteria, the combined system in sunlight should generate H from H2O with a maximum energy conversion efficiency of .apprx.10%.

L20 ANSWER 26 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1984:97724 HCAPLUS

DOCUMENT NUMBER:

100:97724

TITLE:

Quenching the luminescence of luminescent bacteria as

a test for estimating the toxicity of phenol

components of sewage

AUTHOR(S):

Gil, T. A.; Balayan, A. E.; Stom, D. I.

CORPORATE SOURCE:

USSR

SOURCE:

Mikrobiologiya (1983), 52(6), 1014-16

CODEN: MIKBA5; ISSN: 0026-3656

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

Among the 3 tests used for studying the toxicity of wastewater phenols to luminescent bacteria (Beneckea harvey), quenching of the luminescence was most sensitive indicator compared to inhibition of dehydrogenase [9035-82-9] activity and bacterial multiplication. The luminescence quenching was a rapid test with a response time of 10 s, whereas the dehydrogenase and multiplication tests required 6 h and 1 day, resp. The phenols studied could be placed in the decreasing toxicity order (all tests): p-benzoquinone [106-51-4 ], hydroquinone [123-31-9], resorcinol [108-46-3], PhOH [108-95-2]. The quenching of the bacterial luminescence, seen under the effect of the toxicants, can also be observed visually (instead of luminometer used in the actual test); however, the toxicity and accuracy are reduced.

106-51-4, biological studies IT

RL: BIOL (Biological study)

(luminescence quenching by, of bacteria, toxicity in relation

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

L20 ANSWER 27 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1982:609949 HCAPLUS

DOCUMENT NUMBER:

97:209949

TITLE:

Four-hour algal bioassays for assessing the toxicity

of coal-derived materials

AUTHOR(S):

Giddings, J. M.

CORPORATE SOURCE:

Environ. Sci. Div., Oak Ridge Natl. Lab., Oak Ridge,

TN, 37830, USA

SOURCE:

U. S. Environ. Prot. Agency, Off. Res. Dev., [Rep.]

EPA (1981), EPA-600/9-81-018, Proc. Symp. Process

Meas. Environ. Assess., 2nd, 104-16

CODEN: XPARD6; ISSN: 0092-8054

DOCUMENT TYPE:

Report English

LANGUAGE:

Algal cultures or natural algal communities are exposed to coal-derived materials for 4 h. Photosynthesis is determined by the 14C-bicarbonate method during the final 2 h of exposure and compared with controls for a measure of toxicity. In bioassays with individual aromatic compds., quinones, and aromatic amines were particularly toxic to algae; azaarenes, and thiophenes were the least toxic classes tested. Expts. with the water-soluble fractions (WSFs) of >20 natural and synthetic oils showed that coal liquefaction products are considerably more toxic than petroleum products; shale oils are intermediate in toxicity. Further studies with particular subfractions of several SWFs have identified ether-soluble bases as the major contributors to the toxicity of coal-derived oils. The 4-h photosynthesis test has several advantages over the Algal Assay Bottle Test for measuring the toxicity of complex materials.

106-51-4, biological studies IT

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to algae)

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN



L20 ANSWER 28 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1982:449310 HCAPLUS

DOCUMENT NUMBER:

97:49310

TITLE:

A comparison of log P and molecular connectivity in the structure-activity analysis of some antimicrobial

AUTHOR (S):

Boyd, J. C.; Millership, J. S.; Woolfson, A. D.

CORPORATE SOURCE:

Dep. Pharm., Queen's Univ. Belfast, Belfast, BT9 7BL,

SOURCE:

Journal of Pharmacy and Pharmacology (1982), 34(3),

158-61

CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE:

Journal English

LANGUAGE:

Several congeneric series of antimicrobial agents were investigated using mol. connectivity as the descriptor of mol. structure. The fungicidal activity of p-hydroxybenzoates, aliphatic carboxylic acids, benzyl isothiocyanates, and quinones and the antibacterial activity of alkyl  $\beta$ -naphthols and benzyl alcs. were tested. In all cases, mol. connectivity gave comparable or improved correlations with biol. activity compared with the logarithm of the octanol-water coefficient of the mol. (log P). Thus, the use of computer-generated connectivity terms has advantages over the calculated log P values in its ease of application and should be considered at least for initial screening of structure-activity

106-51-4, biological studies 137-18-8 553-97-9 TΤ RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (fungicidal activity of, structure in relation to)

RN 106-51-4 HCAPLUS

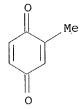
2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

137-18-8 HCAPLUS

2,5-Cyclohexadiene-1,4-dione, 2,5-dimethyl- (9CI) (CA INDEX NAME)

553-97-9 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME) CN



L20 ANSWER 29 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:175979 HCAPLUS

DOCUMENT NUMBER: 96:175979

TITLE: On improvement of garlic productivity by inactivation

of virus in garlics

AUTHOR(S): Lee, Chang Un

CORPORATE SOURCE: Coll. Agric. Anim. Sci., Yeungnam Univ., Gyeongsan,

632, S. Korea

SOURCE: Han'guk Sikmul Poho Hakhoechi (1981), 20(1), 6-14

CODEN: HSHCA8; ISSN: 0367-6285

DOCUMENT TYPE: Journal

LANGUAGE: Korean

The effect of heat or chemotherapeutic treatment on the mosaic AB virus-infected garlic (Allium sativum) scales and that of The chemotherapeutic agents added to the culture medium were studied. treatment of the virus-infected garlic scales at 37.apprx.57% for 35 days to 1 h in water or in air showed no effect on inactivating the virus. Although treatment of the garlic scales at 62.apprx.72° for 90 to 5 min reduced the mosaic symptom of the leaves of the plants grown after the heat treatment, it reduced the growth vigor so greatly that complete inactivation of the virus in garlics was not feasible. The mosaic symptom on the leaves was reduced when the infected garlic scales were grown after 24 h soaking in 10.apprx.50 ppm Malachite Green [569-64-2], 2,4-D [94-75-7], or in 20.apprx.100 ppm Quinhydrone [106-34-3]. These agents, however, inhibited the growth of garlic plant at the high concentration Garlic scales soaked in 10.apprx.50 ppm NAA [86-87-3] showed the least mosaic symptom. When incorporated into the modified Murashige-Skoog's medium, 0.5.apprx.1.5 ppm NAA could inactivate the mosaic virus in newly-developed garlic plants showing no mosaic symptom on the leaves, no inclusion bodies and intact nuclei in the leaf tissue cells.

IT 106-34-3

RL: BIOL (Biological study)
 (mosaic virus control by, in garlic, phytotoxicity in
 relation to)

RN 106-34-3 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, compd. with 1,4-benzenediol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 123-31-9 CMF C6 H6 O2

CM

CRN 106-51-4 CMF C6 H4 O2



HCAPLUS COPYRIGHT 2004 ACS on STN L20 ANSWER 30 OF 44

ACCESSION NUMBER:

1982:117107 HCAPLUS

DOCUMENT NUMBER:

96:117107

TITLE:

Comparison of bacterial luminescence and fish bioassay

results for fossil-fuel process waters and

phenolic constituents

AUTHOR(S):

Lebsack, M. E.; Anderson, A. D.; DeGraeve, G. M.;

Bergman, H. L.

CORPORATE SOURCE:

Alcohol. Res. Treat. Cent., VA Hosp., Bronx, NY,

10468, USA

SOURCE:

ASTM Special Technical Publication (1981), 737 (Aquat.

Toxicol. Hazard Assess.), 348-56 CODEN: ASTTA8; ISSN: 0066-0558

Journal

DOCUMENT TYPE:

LANGUAGE: English

EC50 values (50% luminescence inhibition concentration) using Photobacterium ΔR fischeri (P. phosphoreum) and LC50 (median lethal concentration) for rainbow trout and fathead minnow were similar. For the fossil fuel process waters the luminescence EC50 values were usually within a factor 2 of the fish LC50 values (Paraho 77-78 being a notable exception). A comparison of the bacterial and fish results for phenolic compds. indicates somewhat more variability, but the general toxicity trends are similar. Overall, for all the process waters and phenolic compds., the fish toxicity tests were more sensitive in about half of the cases. This type of toxicity testing system has potential value for semicontinuous monitoring of industrial or municipal effluents.

 $\mathbf{IT}$ 106-51-4, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, bacterial luminescence assay for evaluation of,

fish assay in comparison with)

RN 106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

HCAPLUS COPYRIGHT 2004 ACS on STN L20 ANSWER 31 OF 44

ACCESSION NUMBER:

1981:42246 HCAPLUS

DOCUMENT NUMBER:

94:42246

TITLE:

Evaluation of the mutagenic and toxic action of pulp and paper production wastewater and components on

Drosophila

## Pryor 10 003465

AUTHOR(S):

Grechanyi, G. V.; Zasukhina, O. V.; Nikitin, A. Ya.

CORPORATE SOURCE:

SOURCE:

Issled. Biol. Deistviya Antropogennykh Faktorov,

Zagryaz. Vodoemy (1979), 57-69. Editor(s): Kozhova, O. M. Irkutskii Univ.: Irkutsk, USSR.

CODEN: 44QKAM

DOCUMENT TYPE:

Conference

LANGUAGE:

Russian

GT

Biol. treatment of effluents from the Baikal Paper and Cellulose Combine AB in an aeration pond greatly increased their embryotoxicity to 1 D. melanogaster strain and induced toxicity to another strain which tolerated untreated black and white water, and chemical treated combined effluent. Larvae were raised on a yeast medium spiked with 0.012-1.2 g effluents/L. Replacing wastewaters by 0.012-1.2 g p-quinone [106-51-4] increased the mortality of eggs sired by males raised on I-amended medium. The effluents and I showed no direct toxicity to larvae reared on them. Rearing the less susceptible strain chronically on I eliminated it within 17 generations, whereas the strain more susceptible in the 1st generation survived longer.

L20 ANSWER 32 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1980:631936 HCAPLUS

DOCUMENT NUMBER:

93:231936

TITLE:

Acute and embryo-larval toxicity of phenolic compounds

to aquatic biota

AUTHOR (S):

DeGraeve, G. M.; Geiger, D. L.; Meyer, J. S.; Bergman,

CORPORATE SOURCE:

Dep. Zool. Physiol., Univ. Wyoming, Laramie, WY,

82071, USA

SOURCE:

Archives of Environmental Contamination and Toxicology

(1980), 9(5), 557-68

CODEN: AECTCV; ISSN: 0090-4341

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Because of the prevalence of phenolic compds. in various types of effluents, both acute and embryo-larval bioassays were performed on 8 phenolic compds. with rainbow trout (Salmo gairdneri), fathead minnows (Pimephales promelas), and Daphnia pulicaria. In flow-through bioassays, the 96-h median lethal concentration (LC50) values for rainbow trout and fathead minnows ranged from <0.1 mg/L for hydroquinone [123-31-9] to >100 mg/L for resorcinol [108-46-3]. D. pulicaria Was consistently the least sensitive species tested as measured in 48-h bioassays, while fathead minnows and rainbow trout varied in their relative sensitivity to phenolics as measured in 96-h tests. Fathead minnows were more sensitive to phenol [108-95-2] at 25° than at 14°. In embryolarval bioassays with phenol, fathead minnow growth was significantly decreased by 2.5 mg/L, while rainbow trout growth was significantly decreased by 0.20 mg/L. For both species, the embryolarval effects concentration was 1.1% of the 96-h LC50. Another embryolarval bioassay was attempted with p-benzoquinone [ 106-51-4], a highly toxic phenolic compound found in fossil fuel processing wastewaters, which was discontinued because the compound was rapidly degraded chemical or biol. in the headtank and aquaria.

106-51-4, biological studies IT

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to aquatic biota)

106-51-4 HCAPLUS RN

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

HCAPLUS COPYRIGHT 2004 ACS on STN L20 ANSWER 33 OF 44

ACCESSION NUMBER:

1980:562090 HCAPLUS

DOCUMENT NUMBER:

93:162090

TITLE:

The disposition of aromatic hydrocarbons in adult spot shrimp (Pandalus platyceros) and the formation of metabolites of naphthalene in adult and larval spot

shrimp

AUTHOR (S):

Sanborn, H. R.; Malins, D. C.

CORPORATE SOURCE:

Northwest Alaska Fish. Cent., NOAA, Seattle, WA,

98112, USA

SOURCE:

Xenobiotica (1980), 10(3), 193-200

CODEN: XENOBH; ISSN: 0049-8254 Journal

DOCUMENT TYPE:

English

LANGUAGE:

AΒ Adult spot shrimp exposed to 110 ppb of the water-soluble fraction of Prudhoe Bay crude oil for 1 wk accumulated a variety of low-mol.-weight aromatic hydrocarbons (primarily C1-C5 substituted derivs.) in thoracic and abdominal tissues. In adult shrimps exposed to 14C- and 3H-labeled naphthalene [91-20-3] in seawater, nonconjugated derivs. (quinone **106-51-4**],  $\alpha$ -naphthol [90-15-3], and naphthalene-1,2dihydrodiol [7234-04-0]) represented 69% of the total conversion products, conjugated metabolites (sulfate, glucuronide, and glycoside) each accounted for ≤7%, and an unidentified metabolite accounted for 16% of the total conversion products. Larval shrimps exposed to naphthalene showed different compns.; naphthyl sulfate [69206-01-5] and naphthol represented 39 and 44%, resp., of the total conversion products and quinone and dihydrodiol represented small percents (7 and 4%, resp.).

L20 ANSWER 34 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1980:401667 HCAPLUS

DOCUMENT NUMBER:

93:1667

TITLE:

Effect of phenols of wastewaters on some

energy-dependent parameters of Chaveal alga cells AUTHOR(S): Plekhanov, S. E.; Stom, D. I.; Khitrov, Yu. A.;

Yasinovskii, V. G.

CORPORATE SOURCE:

Mosk. Gos. Univ., Moscow, USSR

SOURCE:

Biologicheskie Nauki (Moscow) (1980), (2), 40-3

CODEN: BINKBT; ISSN: 0303-4119

DOCUMENT TYPE:

LANGUAGE:

Journal Russian

GI

AB The effects of PhOH [108-95-2], hydroquinone (I) [123-31-9], p-benzoquinone [106-51-4], resorcinol [108-46-3], pyrocatechol [120-80-9], and guaicol [90-05-1] was examined on the isolated internodal cells of Nitella growing in wastewater (during various stages of purification). The phenols inhibited the rate of cytoplasmic movement. At 1 + 10-3 and 5 + 10-4M, they reduced the elec. p.d. at the plasmalemma and increased the elec. resistance. A further increase in the concentration of the phenols caused an irreversible decrease in these changes and finally cell death. Changes in the p.d. and elec. resistance, shown by the plasmalemma at low concns. of phenols, may be useful criteria to evaluate the toxicity of phenols.

IT 106-51-4, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to algae, elec. activity in relation to)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L20 ANSWER 35 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:16515 HCAPLUS

DOCUMENT NUMBER: 92:16515

TITLE: Acute toxicity to Selenastrum capricornutum of

aromatic compounds from coal conversion

AUTHOR(S): Giddings, Jeffrey M.

CORPORATE SOURCE: Environ. Sci. Div., Oak Ridge Natl. Lab., Oak Ridge,

TN, 37830, USA

SOURCE: Bulletin of Environmental Contamination and Toxicology

(1979), 23(3), 360-4

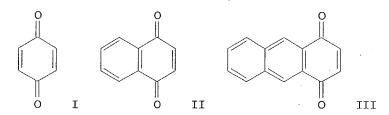
CODEN: BECTA6; ISSN: 0007-4861

CODEN: DECIMO; 155N: UUU/-40

DOCUMENT TYPE: Journal

LANGUAGE: English

GΙ



AB In freshwater alga (S. capricornutum) exposed to coal-derived aromatic compds. at concns. of 10, 100 and 1000 mg/L (soluble compds.) or at 1, 10 and 100% saturation (compds. whose solubility was <1000 mg/L), p-benzoquinone (I) 106-51-4] and 1,4-naphthoquinone (II) [130-15-4] were the most toxic compds., based on short-term photosynthetic inhibition as the measure of toxic response. 1,4-Anthraquinone (III) [635-12-1] was essentially nontoxic to the algae, as were all the other 3-ring

compds. except acridine [260-94-6]. Aromatic amines (aniline [62-53-3] and 1-naphthylamine [134-32-7]) were highly toxic as was 2-naphthol [135-19-3]. Thiophenes and azaarenes were only slightly toxic except at the highest concns. The other classes of aromatic compds. (methylated aroms. and hydrocarbons) were intermediate in toxicity. An all cases, 2-ring compds. were more toxic than related 1-ring compds.

ANSWER 36 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1978:165148 HCAPLUS

DOCUMENT NUMBER:

88:165148

TITLE:

Possible mechanism of action of quinone pesticides on

the protoplasmic streaming in marine plants

AUTHOR(S):

SOURCE:

Stom, D. I.; Rogozina, N. A.

CORPORATE SOURCE:

Biol.-Geogr. Nauchno-Issled. Inst., Irkutsk, USSR Eksperimental'naya Vodnaya Toksikologiya (1976), 6,

111-18

CODEN: EKVTA6; ISSN: 0367-0724

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian Cessation of protoplasmic streaming in Nitella and Elodea canadensis was

an earlier indicator of damage from phenols (such as hydroquinone [123-31-9] and resorcinol [108-46-3]) and quinones (including

p-benzoquinone [106-51-4] and  $\beta$ -naphthoquinone

[524-42-5]) than was plasmolysis and deplasmolysis. phenols oxidizable to quinones also inhibited ATPase [9000-83-3] activity. A possible mechanism for the damaging effect of quinone pesticides on protoplasm streaming is blocking of the -SH groups and inactivation of the thiol enzymes, especially ATPase.

L20 ANSWER 37 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1978:70423 HCAPLUS

DOCUMENT NUMBER:

88:70423

TITLE:

A new degradation product of the insecticide

mexacarbate found in fresh water

AUTHOR(S):

Roberts, Richard B.; Look, Melvin; Haddon, William F.;

Dickerson, Thomas C.

CORPORATE SOURCE:

Pac. Southwest Forest Range Exp. Stn., Forest Serv.,

Berkeley, CA, USA

SOURCE:

Journal of Agricultural and Food Chemistry (1978),

26(1), 55-9

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE:

Journal

LANGUAGE:

English

O2CNHMe Me  $NMe_2$ Ι

The carbamate insecticide mexacarbate (I) [315-18-4] was degraded in AΒ plants and animals by oxidation of the dimethylamino group and by hydrolysis of the carbamate moiety. In water solns. of different pH

## Pryor 10 003465

values, essentially the same degradation products were found: 4-methylamino-3,5-xylyl methylcarbamate [10389-50-1], 4-amino-3,5-xylyl methylcarbamate [831-76-5], 4-methylformamido-3,5-xylyl methycarbamate [10233-94-0], 4-formamido-3,5-xylyl methylcarbamate [10233-95-1], and 4-dimethylamino-3,5-xylyl hydroxymethylcarbamate [10310-18-6]. Additional products identified included 4-dimethylamino-3,5-xylenol [6120-10-1] and 2-hydroxy-3,5-dimethyl-p-benzoquinone [2913-40-8 ], a new degradation product. Bioassay of this new degradation product on sixth stage western spruce budworm (Choristoneura occidentalis) larvae indicated little or no toxicity at the rate of 0.1 mg/g by topical application and 0.05 mg/g by injection.

L20 ANSWER 38 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1976:588993 HCAPLUS

DOCUMENT NUMBER:

85:188993

TITLE:

Study of the photoreduction of exogeneous electron acceptors by blue-green algae. Mediator mechanism of

electron transport through a biomembrane

Varfolomeev, S. D.; Zaitsev, S. V.; Belogurova, N. G.;

Berezin, I. V.; Nikitina, K. A.; Gusev, M. V.

Chem. Dep., M. V. Lomonosov State Univ., Moscow, USSR CORPORATE SOURCE:

Bioorganicheskaya Khimiya (1976), 2(10), 1395-403 SOURCE:

CODEN: BIKHD7; ISSN: 0132-3423

DOCUMENT TYPE:

Journal Russian

LANGUAGE:

ΤТ

AUTHOR(S):

In the blue-green algae Anabaena variabilis and Anacystis nidulans, the

photoredn. of K ferricyanide took place only in the presence of

p-benzoquinone. The photoredn. reaction is inhibited by

 $ar{3}$ -(3,4- $ar{d}$ ichlorophenyl-1,1-dimethylurea), this fact being indicative of the water splitting system participation in the process. A mechanism

is suggested to account for p-benzoquinone effects, which involves the stages of photoredn. of p-benzoquinone and electron transport through a

biomembrane onto K ferricyanide. 106-51-4, biological studies

RL: BIOL (Biological study)

(in photoredn. of potassium ferricyanide with blue-green algae

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

L20 ANSWER 39 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1966:22699 HCAPLUS

DOCUMENT NUMBER:

64:22699

ORIGINAL REFERENCE NO.:

64:4201g-h,4202a-b

Fungicides containing di-, tri-, and

tetramethyl-1,4-benzoquinone monooxime and

water-soluble salts thereof

PATENT ASSIGNEE(S):

United States Rubber Co.

SOURCE:

9 pp. Patent

DOCUMENT TYPE:

Unavailable

LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO.

DATE

NL 6413711

PRIORITY APPLN. INFO.:

BY 19631230

AB The fungicides are especially suitable to apply to the soil to protect seeds and sprouting plants against especially Rhizoctonia solani, using preferably 0.28-5.6 kg./ha. on seed rows of a width of 5 cm. and a depth of 5 cm. and 1 m. apart, or using 11.2-224 kg./ha. when spraying on all of the soil. A powdered composition for spraying consists, e.g., of 2,5-dimethyl-1,4-benzoquinone monooxime (I) 75, Dixie Clay (kaolin) 12, Polyfon H (Na lignosulfonate) 2, Triton X-120 5, and ethylene glycol 6 parts, and preferably 0.1-3 parts powdered carrier as clay or mineral silicates per part active ingredient. In

testing the fungicidal activity in cotton plants, 66 mg. was mixed with 450 g. sand. The premixt. was mixed with 28.5 kg. earth to obtain a concentration of 20 ppm. The mixture was put in pots (diameter 10 cm.), after which

cotton seeds "Fox-4" were put on the soil. A grain of oats infected with R. solani of a culture 2 weeks old, was put between the cotton seeds in 5 pots. In comparison 5 seeds were put in 5 pots containing untreated earth without the infected grain of oats and the same with the infected grain of oats. The seeds were covered with a 1.25-cm. layer of earth. The pots were kept at 22-6° in a moist atmospheric After 2 and 3 weeks the percent of surviving plants based on sprouted plants was determined Results are given in the table. %, sprouted, plants, %, surviving, plants; I 20 ppm., 80, 76; 2,6-dimethyl-1,4-benzoquinone monooxime 20 ppm., 84, 76; untreated infected earth, 76, 0; untreated noninfected earth, 92, 92; 2,3,5-trimethyl-1,4-benzoquinone monooxime 20 ppm., 72, 68; 2,3,5,6-tetramethyl-1,4-benzoquinone monooxime 80, , ; ppm., 80, 76; untreated infected earth, 42, 0; untreated noninfected earth, 88, 88; I 20 ppm. + tetramethylthiuram disulfide (II) 20, , ; ppm., 82, 93; I 10 ppm. + II 20 ppm., 82, 66; untreated infected earth, 86, 7; untreated noninfected earth, 84, 98;

IT 30554-01-9, p-Benzoquinone, 2,6-dimethyl-, oxime

KIND

DATE

(as fungicide)

RN 30554-01-9 HCAPLUS

CN p-Benzoquinone, 2,6-dimethyl-, monooxime (8CI) (CA INDEX NAME)

CM 1

PATENT NO.

CRN 7803-49-8 CMF H3 N O

 $H_2N-OH$ 

CM 2

CRN 527-61-7 CMF C8 H8 O2

IT 106-51-4, p-Benzoquinone

(derivs., as fungicides)

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

L20 ANSWER 40 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1957:57399 HCAPLUS

DOCUMENT NUMBER:

51:57399

ORIGINAL REFERENCE NO.:

51:10663d-e

TITLE:

Pristimerin III. Antibacterial activity of some simple

orthoquinones

AUTHOR(S):

Kamat, V. N.; de Sa, J.; Fernandes, F.; Bhatnagar, S.

CORPORATE SOURCE:

St. Xavier's Coll., Bombay

SOURCE:

J. Sci. Ind. Research (India) (1956), 15C, 8-9

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

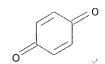
Only the o-quinones were active against organisms of the viridans group. An increase in the water solubility of quinones and in the number of rings present in the mol. decreases activity. 1,2-Benzoquinone, 1,2-naphthoquinone, 4-amino-1,2-naphthoquinone, and 9,10-phenanthraquinone (I) show 2.5-12.5 times the activity of pristimerin (II) against Micrococcus pyogenes var. aureus, (III), Diplococcus pneumoniae, type II, Streptococcus pyogenes, and S. viridans I with the exception that I is equal but not superior to II in its activity against III.

106-51-4, p-Benzoquinone IT

(effect on bacterial growth)

RN106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN



L20 ANSWER 41 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1948:4697 HCAPLUS

DOCUMENT NUMBER:

42:4697

ORIGINAL REFERENCE NO.: 42:1014e-f

TITLE:

Derivatives of halogenated quinones as fungicides

INVENTOR(S):

Ladd, Elbert C.; Harvey, Merlin P.

PATENT ASSIGNEE(S):

U.S. Rubber Co.

DOCUMENT TYPE:

Patent

LANGUAGE:

Unavailable

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE PATENT NO. KIND DATE \_ \_ \_ \_ \_ \_ \_\_\_\_\_ US 2430722 19471111 US

Derivs. of tetrachloro-(I) and tetrabromo-p-quinone and of 2,3-dichloro-AB and 2,3-dibromo-1,4-naphthoquinone, obtained by replacement of one of the

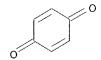
## Pryor 10 003465

halogens by the residue obtained by removing a H from a compound containing an active -CH2-, are fungicides. Thus the diethyl ester of 3,5,6-trichloro-1,4-benzoquinone-2-oxalacetic acid, m. 102-3.5°, from EtOH was prepared, by addition of 3 mols. of (CH:CONa) (CO2Et)2 to 1 mol. I in acetone. After 1.5 hrs., the solution was filtered, acidified with HCl, diluted with water, and the solid recrystd. Cf. C.A. 39, 1246.4; 41, 5899h, 5900a.

IT 106-51-4, p-Benzoquinone
 (derivs., for fungicides)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L20 ANSWER 42 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1947:31250 HCAPLUS

DOCUMENT NUMBER: 41:31250
ORIGINAL REFERENCE NO.: 41:6302a-c

TITLE: Routine examination for antibiotics produced by molds

AUTHOR(S): Heatley, N. G.; Philpot, Flora J.

CORPORATE SOURCE: Univ. of Oxford

SOURCE: Journal of General Microbiology (1947), 1, 232-7

CODEN: JGMIAN; ISSN: 0022-1287

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB Routine performance of a few simple tests on culture filtrates of antibiotic-producing fungi serves to identify presumptively the presence of any of the following 14 antibiotics; penicillin, helvolic acid, mycophenolic acid, proactinomycin, citrinin, gliotoxin, puberulic acid, fumagatin, spinulosin, patulin (clavacin), aspergillic acid, penicillic acid, kojic acid and streptomycin. The tests are: stability at pH 2.0 and 9.5; ether-water partition at pH 2.0, 6.0-7.0 and 9.0; relative activities towards specified strains of Staphylococcus aureus and Escherichia coli, destruction by penicillinase, color reactions and volatility with steam. In some cases it may be essential to isolate the inhibitor and characterize it by the usual chemical criteria.

IT 85-23-4, Spinulosin

(from molds)

RN 85-23-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3-methoxy-6-methyl- (9CI) (CA INDEX NAME)

L20 ANSWER 43 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1946:37655 HCAPLUS

## Pryor 10 003465

DOCUMENT NUMBER:

40:37655

ORIGINAL REFERENCE NO.:

40:7277c-d

TITLE:

The antibiotic action in vitro of naphthoguinone and

of synthetic water-soluble vitamin K against staphylococcus, B. diphtheriae, and B. typhi

AUTHOR (S):

Nassi, Lelio

CORPORATE SOURCE:

Univ. Florence, Italy

SOURCE:

Bollettino - Societa Italiana di Biologia Sperimentale (1946), 21, 141-4

CODEN: BSIBAC; ISSN: 0037-8771

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

Naphthoquinone (0.04%) and 2-methyl-1,4-disuccinylnaphthoquinone (0.1%) AB

show antibiotic activity, particularly against staphylococcus.

106-34-3, Quinhydrone 106-51-4, Quinone IT

(bactericidal action of)

106-34-3 HCAPLUS RN

CN 2,5-Cyclohexadiene-1,4-dione, compd. with 1,4-benzenediol (1:1) (9CI) (CA

ÍNDEX NAME)

CM1

CRN 123-31-9 CMF C6 H6 O2

OH

CM

CRN 106-51-4 CMF C6 H4 O2

106-51-4 HCAPLUS RN

CN2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L20 ANSWER 44 OF 44 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1919:8838 HCAPLUS

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.:

13:8838 13:1718f-i

TITLE:

Some factors influencing the effect of dyes and allied

compounds on bacteria

AUTHOR(S):

Graham-Smith, G. S.

SOURCE:

Journal of Hygiene (1919), 18, 1-32

CODEN: JOHYAY; ISSN: 0022-1724

DOCUMENT TYPE:

Journal

LANGUAGE: Unavailable

In cultures the effects of homoflavine and quinone, the compds. most thoroughly investigated, vary on each species of organism with each change of composition of the medium, whether the change is brought about by altering the proportion of any constituent, or by adding new constituents, and also with variations in the number and age of the organism. In each medium the concentration of the compound which inhibits each species differs, and it is probable that still other concns. are required when mixed cultures are used, though this is not established by experiment. In wounds the conditions are more complex than in cultures. The conditions in no two wounds are likely to be identical, and are constantly altering, in chemical composition, number of species, and interrelationships of organisms. S. concludes as follows: A wound must be thoroughly cleansed before the application of the dye since the complex organic fluids present may interfere with the action of the solution The compound should be dissolved in a fluid with the optimum reaction for that substance if such a reaction is not harmful to the tissues. Some compds. are more efficient than others against certain species of bacteria. Compds. are more effective in the early stages of an infection since the organisms later increase in number, become accustomed to their surroundings, and are protected in the fluids. It would be desirable to test the action on wounds of a solution in distilled water of 1:10000 hemoflavine, 1:10000 quinone, 1:100000 crystal violet. Some good results have been obtained in pyorrhea, stomatitis, and gingivitis. Plates and references are given.

IT 106-51-4, Quinone

(effect on bacteria)

RN106-51-4 HCAPLUS

CN2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

=> N

L19

L20

=> d stat que nos

L7

L9 SCR 1839

L114180 SEA FILE=REGISTRY SSS FUL L7 NOT L9

L14STR

L15 901 SEA FILE=REGISTRY SUB=L11 SSS FUL L14

16802 SEA FILE=HCAPLUS ABB=ON PLU=ON L15

L16 L1821 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L)(?PORIFER? OR ?HELMINTH? OR ?COELOMA? OR ?ANNELID? OR ?WORM? OR ?MOLLUSK? OR ?BIVAL? OR ?LARV? OR ?COPEPOD? OR ?OSTRACOD? OR ?MYSID? OR ?GAMMARID?

OR ?DECAPOD? OR ?TELEOS? OR ?STARFISH?)

361 SEA FILE=HCAPLUS ABB=ON PLU=ON L16(L) (PEST? OR AQUACID? OR ?VIRUS? OR ?PROTI? OR ?FUNGI? OR MOLD OR MOLDS OR ANTIMOLD OR ?PLANKTON? OR ?DEMERS? OR ?BENTHI? OR ?BIOTA? OR ?BACTER? OR ?PROTOZO? OR ?ALGAE? OR ?PYRROP? OR ?CRYPTOP? OR ?CHRYSOPH?)

44 SEA FILE=HCAPLUS ABB=ON PLU=ON (L18 OR L19) AND (WATER OR

AQUA?)

3 SEA FILE=HCAPLUS ABB=ON PLU=ON ((L18 OR L19) AND (MARIN? OR T<sub>2</sub>1

#### SEAWATER)) NOT L20

=> =>

=> d ibib abs hitstr l21 1-3

L21 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2004:568535 HCAPLUS

DOCUMENT NUMBER:

141:84034

TITLE:

Bactericides for marine periphytic bacteria

containing natural products, and method and agent for

controlling bioadhesion of marine organisms

to ship bottom

INVENTOR(S):

Ishii, Akira; Kohiyori, Hideki; Makita, Yoji; Umeno,

Aya; Oi, Kenta

PATENT ASSIGNEE(S):

National Institute of Advanced Industrial Science and

Technology, Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004196677	A2	20040715	JP 2002-364508	20021217
PRIORITY APPLN. INFO.:			JP 2002-364508	20021217
AB The bactericides,	which	control marine	periphytic bacteria,	thus

The bactericides, which control marine periphytic bacteria, thus preventing biofouling of barnacle larvae, etc., contain ≥1 selected from organism exts., spices, polysaccharides, organic acids, and proteins. Adhesion of marine organisms is prevented by coating ship bottoms with paints containing ≥1 of the above components optionally adsorbed by carriers. Thus, hinokitiol (I) inhibited growth of Pseudoalteromonas carrageenovora. Antifouling effect of a paint containing I on a ship bottom was also shown.

IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); TEM (Technical or engineered material use); BIOL (Biological study); USES (Uses)

(bactericides for marine periphytic

bacteria containing organism exts., spices, polysaccharides, organic acids, or proteins, and their use for ship bottom antifouling paints)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L21 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:561826 HCAPLUS

DOCUMENT NUMBER:

122:287292

TITLE:

Inhibitory effect of bacterial ubiquinones on the

settling of barnacle, Balanus amphitrite

AUTHOR(S):

Kon-ya, K.; Shimidzu, N.; Otaki, N.; Yokoyama, A.;

Adachi, K.; Miki, W.

Shimizu Laboratories, Marine Biotechnology Institute CORPORATE SOURCE:

(MBI), Shizuoka, 424, Japan

Experientia (1995), 51(2), 153-5 SOURCE:

CODEN: EXPEAM; ISSN: 0014-4754

Birkhaeuser PUBLISHER: Journal DOCUMENT TYPE: English LANGUAGE:

> In an attempt to clarify the influence of marine bacteria on the settling of fouling invertebrate larvae, we screened for inhibitors,

produced by marine bacteria, of settling by cyprids of the

barnacle, Balanus amphitrite. We found that the culture broth of Alteromonas sp. strain number KK10304, which was associated with the marine sponge, Halichondria okadai, effectively inhibited settling of the cyprids. Bioassay-guided isolation indicated ubiquinone-8 as an effective inhibitor of cyprid settling. As ubiquinones are widely distributed in bacteria, several related compds. were also tested. 605-94-7, Ubiquinone-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(ubiquinones from bacteria associated with marine sponge inhibition of settling of barnacle larvae)

605-94-7 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX CNNAME)

AΒ

TT

L21 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:666976 HCAPLUS

DOCUMENT NUMBER: 119:266976

Organohalogen constituents of the acorn worm TITLE:

Ptychodera bahamensis

Corgiat, Jay M.; Dobbs, Fred C.; Burger, Mike W.; AUTHOR (S):

Scheuer, Paul J.

Dep. Chem., Univ. Hawaii, Honolulu, HI, 96822, USA CORPORATE SOURCE:

Comparative Biochemistry and Physiology, Part B: SOURCE:

Biochemistry & Molecular Biology (1993), 106B(1), 83-6

CODEN: CBPBB8; ISSN: 0305-0491

DOCUMENT TYPE: Journal

English LANGUAGE:

Twenty organohalogen compds., primarily phenols, were detected in the volatile exts. of the acorn worm Ptychodera bahamensis. Five chlorinated compds., previously undescribed from acorn worms, were identified.

Enteropneusts can be significant contributors of halogenated orgs. to the marine environment.

29533-24-2, Dibromoquinone IT RL: BIOL (Biological study)

(in acorn worm)

29533-24-2 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, dibromo- (9CI) (CA INDEX NAME) CN

2 (D1-Br)

=> 🗆

T<sub>2</sub>5

=> d his 125

(FILE 'HCAPLUS' ENTERED AT 16:20:04 ON 06 DEC 2004) 36 S (L23 AND L24) NOT (L20 OR L21)

=> d ibib abs hitstr 125 1-36

L25 ANSWER 1 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:710474 HCAPLUS

DOCUMENT NUMBER: 141:391785

TITLE: Quinones as antimycobacterial agents

AUTHOR(S): Tran, Thuyanh; Saheba, Ekta; Arcerio, Ariana V.;

Chavez, Violeta; Li, Qing-yi; Martinez, Luis E.;

Primm, Todd P.

CORPORATE SOURCE: Department of Biological Sciences, The University of

Texas at El Paso, El Paso, TX, 79968, USA

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(18),

4809-4813 CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

Mycobacterium tuberculosis is a serious worldwide health threat, killing almost 3 million people per yr. Other mycobacterial species, especially Mycobacterium avium, are emerging pathogens in the immunocompromised population, most notably AIDS patients. These nontuberculous mycobacteria (NTM) are ubiquitous in the environment, and naturally resistant to many disinfection procedures. Treatment options are limited, and no new antibiotics have been developed against mycobacteria since the 1970s. There is a desperate need for new biocides and antibiotics to prevent and treat mycobacterial infections. A small aromatic compound library has been screened for effectiveness in growth inhibition or killing of mycobacteria. Four species, representing the M. tuberculosis complex, the slow-growing NTM, and the rapid-growing NTM were used. Active compds. had minimal inhibitory concns. as low as 12.5 µg/mL, with the active component being a quinone. The primarily bactericidal activity observed represents a unique mechanism of action. A fluorescent assay involving M. smegmatis expressing gfp was analyzed as a rapid assay for predicting inhibitory activity, but failed to predict activity well. Thus, these compds. may have significant utility as soluble biocides against mycobacteria and other hardy nosocomial pathogens.

IT 106-51-4, 1,4-Benzoquinone, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(quinones as antimycobacterial agents)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:362583 HCAPLUS

DOCUMENT NUMBER: 141:106252

TITLE: Synthesis and evaluation of novel 1,4-naphthoquinone

derivatives as antiviral, antifungal and anticancer

agents

AUTHOR(S): Tandon, Vishnu K.; Singh, Ravindra V.; Yadav,

Dharmendra B.

CORPORATE SOURCE: Department of Chemistry, Lucknow University, Lucknow,

226007, India

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),

14(11), 2901-2904

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:106252

GΙ

$$\begin{array}{c|c} O & & \\ \hline & S & \\ \hline & O & \\ \hline & O & \\ \hline & O & \\ \end{array}$$

AB The synthesis and evaluation of some 2-substituted-1,4-naphthoquinones, S-(1,4-naphthoquinon-2-yl)mercaptoalkanoic acid amides, e.g., I, and related quinone derivs., were carried out. The antifungal, antibacterial, antiviral, and anticancer activities were determined by using the standard assay. The results showed that a few of the compds. showed in vitro antiviral activity against Inflenza-A Virus and Herpes Simplex Virus and possess pronounced antifungal profile whereas I showed anticancer activities against Lymphoid Leukemia P 388.

IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, antifungal, and antibacterial activity of carboxypropylsulfanyl- and carboxyphenylsulfanylguinone

Ι

carboxypropylsulfanyl- and carboxyphenylsulfanylquinones via condensation of quinones with mercaptopropanoic or mercaptobenzoic acids)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2004:146768 HCAPLUS

DOCUMENT NUMBER:

140:350028

TITLE:

Designing Antibacterial Compounds through a

Topological Substructural Approach

AUTHOR(S):

Molina, Enrique; Gonzales Diaz, Humberto; Gonzalez, Maykel Perez; Rodriguez, Elismary; Uriarte, Eugenio Department of Chemistry and Pharmacy Faculty of

CORPORATE SOURCE:

Engineering Chemistry and Pharmacy, University of

Camagueey, Camagueey, 74650, Cuba

SOURCE:

Journal of Chemical Information and Computer Sciences

(2004), 44(2), 515-521

CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE: English

A novel application of TOPol. Substructural Mol. DEsign (TOPS-MODE) was carried out in antibacterial drugs using computer-aided mol. design. Two series of compds., one containing antibacterial and the other containing non-antibacterial compds., were processed by a k-means cluster anal. in order to design training and predicting series. All clusters had a p-level < 0.005. Afterward, a linear classification function has been derived toward discrimination between antibacterial and non-antibacterial compds. The model correctly classifies 94% of active and 86% of inactive compds. in the training series. More specifically, the model showed a global good classification of 91%, i.e., 263 cases out of 289. predicting series, the model has shown overall predictabilities of 91 and 83% for active and inactive compds., resp. Thereby, the model has a global percentage of good classification of 89%. The TOPS-MODE approach, also, similarly compares with respect to one of the most useful models for antimicrobials selection reported to date.

TΤ 85-23-4 484-89-9, Fumigatin

> RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(designing antibacterial compds. through a topol.

substructural approach)

RN 85-23-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3-methoxy-6-methyl- (9CI) INDEX NAME)

Me<sub>0</sub> HO

484-89-9 HCAPLUS RN

CN 2,5-Cyclohexadiene-1,4-dione, 3-hydroxy-2-methoxy-5-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

CORPORATE SOURCE:

2004:2006 HCAPLUS

DOCUMENT NUMBER:

141:54149

TITLE:

Chemoselective reaction of bisheterocycle

dicarboxylate towards hydrazine hydrate: Synthesis and antimicrobial activity of some new trisheterocycles: 5-pyrrolylaminocarbonyl/oxadiazolyl/mercaptooxadiazoly

lmethoxy-1-furfuryl-2-methylindoles

AUTHOR(S):

Gadaginamath, Guru S.; Donawade, Dundappa S. Post Graduate Department of Chemistry, Karnatak

University, Dharwad, 580 003, India

SOURCE:

Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2003),

42B(12), 3108-3112

CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER:

National Institute of Science Communication

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 141:54149

GΙ

## \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

- AB Chemoselectivity of C5-ester over C3-carbethoxy ester function of the bisheterocycle dicarboxylate I (R = OMe) towards the nucleophilic attack of hydrazine hydrate has been evidenced by the exclusive formation of monohydrazide I (R = NH2NH), which was further reacted with acetonyl acetone, tri-Et orthoformate or carbon disulfide to furnish pyrrolylaminocarbonyl/oxadiazolyl/mercaptooxadiazolylmethoxy furfurylindoles II-IV, resp. The newly synthesized compds. were screened for their antibacterial and antifungal activities.
- IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, reactions RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of furfurylindoles as antibacterial and antifungal agents via chemoselective nucleophilic substitution of furfurylindole dicarboxylate with hydrazine followed by cyclocondensation with hexanedione, orthoester or carbon disulfide)

RN 106-51-4 HCAPLUS

.CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



SOURCE:

REFERENCE COUNT:

RECORD. ALL CITATIONS AVAILABLE

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

25

ACCESSION NUMBER: 2002:934746 HCAPLUS

DOCUMENT NUMBER: 138:351053

TITLE: Benzoquinone, the substance essential for

antibacterial activity in aqueous extracts from succulent young shoots of the pear Pyrus spp.

AUTHOR(S): Jin, Shigeki; Sato, Norio

CORPORATE SOURCE: National Agricultural Research Center for Hokkaido

Region, Toyohira-ku, Sapporo, 062-8555, Japan Phytochemistry (Elsevier) (2003), 62(1), 101-107

CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

Aqueous exts. of the tissue of succulent young shoots of the pear Pyrus spp. exhibited strong antibacterial activity against the bacterium Erwinia amylovora bv. 4. This activity was investigated quant. by a newly developed bioassay method. It was found that the activity changed with the age of the tissue. Exts. of the youngest leaves and stems from the shoot tops showed the stronges't activity, and the activity decreased with age of the leaves and stems. The activity also changed with increase in time after preparation of the extract, increasing rapidly in the first hour after preparation, reaching a maximum at about 4 h, and then decreasing slowly. substance essential for the antibacterial activity was isolated from the extract by steam distillation in vacuo and through charcoal powder column chromatog. It was identified as benzoquinone (2,5-cyclohexadiene-1,4dione) by NMR-spectra, mass spectra and HPLC anal. The phenolic metabolism from arbutin to hydroquinone and then to benzoquinone in the aqueous exts. was analyzed quant. by HPLC. The changes in the contents of benzoquinone in the exts. of leaves and stems with tissue aging and with increase in time after preparation of the exts. paralleled the changes in antibacterial activity as determined by the quant. bioassay.

IT 106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies
RL: BSU (Biological study, unclassified); NPO (Natural product
occurrence); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(benzoquinone is essential for antibacterial activity in
Pyrus ussuriensis exts.)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 6 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 2002:658133 HCAPLUS

DOCUMENT NUMBER:

137:185762

TITLE:

Preparation of aminodeoxy disaccharide bicyclic derivatives of leucomycins as antibacterial agents

INVENTOR(S):

Or, Yat Sun; Binet, Sophie; Phan, Ly Tam

PATENT ASSIGNEE(S):

Enanta Pharmaceuticals, Inc., USA

SOURCE:

PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PA.	rent 1	NO.			KINI	0	DATE			APPL:	ICAT	ION 1	NO.		D	ATE	
	WO	2002	0664	87		A1	_	2002	 0829		WO 2	 002-1	US14:	27		2	0020	117
		W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	ВB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DΖ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JΡ,	KΕ,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,_	NO,	NZ,	OM,	PH,
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SΙ,	SK,	SL,	ТJ,	TM,	TR,	TT,	ΤZ,	UA,
			UG,	UΖ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,
			CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,
			BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
	US	6462	026			B1		2002	1008		US 2	001-	7857	27		2	0010	216
	US	2002	1609	66		A1		2002	1031									
PRIC	ORIT	Y APP	LN.	INFO	. :						US 20	001-	7857	27	i	A 2	0010	216
OTHE	ER SO	OURCE	(S):			MAR	PAT	137:	1857	52								
GT																		

Bicyclic leucomycins, e.g. I, were prepared wherein A is CHO, protected AB aldehyde, CH2X, X is halogen, amine, amino-carbonyl, sulfonyl, aryloxy, heterocycle-oxy, alkoxy, alkenyloxy, alkynyloxy, heterocycle; B and Q are independently H, ester, acyl, amide, CH2X, CN, CHO, alkyl, alkenyl, alkynyl; B and Q together are -C(O)YC(O)-; Y is O, substituted C or N; R is H, hydroxy protecting group; R1 and R2 are independently H, OH, protected hydroxy, ester, D-forosamine, L-mycarose; R3 and R4 are independently H, hydroxy protecting group, acyl, and pharmaceutically acceptable compns. comprising a therapeutically effective amount of a compound of the invention in combination with a pharmaceutically acceptable carrier, a method for treating bacterial infectious by administering to a mammal (no data). Thus, I [A = CHO, R = R1 = R3 = H; R2 = Ac, R4 = R4]C(O)CH2CH(Me)2, B and Q taken together are C(O)N(Ph)C(O)] was prepared as antibacterial agent (no data).

106-51-4, 1,4-Benzoquinone, reactions IT

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of aminodeoxy disaccharide bicyclic derivs. of leucomycins as antibacterial agents)

106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

REFERENCE COUNT:

CORPORATE SOURCE:

RN

CN

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 7 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:50135 HCAPLUS

DOCUMENT NUMBER: 137:6102

Studies on quinones. Part 35: Access to antiprotozoal TITLE:

active euryfurylquinones and hydroquinones

AUTHOR (S): Valderrama, Jaime A.; Benites, Julio; Cortes, Manuel;

Pessoa-Mahana, David; Prina, Eric; Fournet, Alain

Facultad de Quimica, Pontificia Universidad Catolica

de Chile, Santiago, Chile

Tetrahedron (2002), 58(5), 881-886 SOURCE:

CODEN: TETRAB; ISSN: 0040-4020

Elsevier Science Ltd. PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

CASREACT 137:6102 OTHER SOURCE(S):

(+)-Euryfuran adds regiospecifically to activated monosubstituted 1,4-benzoquinones under mild conditions to give the corresponding Michael adducts which, depending on the quinone substituent, undergo in situ redox reactions to the resp. euryfurylbenzoquinones. One of these Michael adducts undergoes a facile stereoselective cyclisation under oxidant conditions to afford a naphthofuro[4,3-c]benzopyran derivative The in vitro activities of the obtained euryfurylquinones and hydroquinones against Leishmania amazonensis are described. The compds. thus prepared and tested included (+)-3,6-dihydroxy-2-[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-6,6,9atrimethylnaphtho[1,2-c]furan-3-yl]benzaldehyde, (-)-1-[3,6-dihydroxy-2-[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-6,6,9a-trimethylnaphtho[1,2-c]furan-3-y1]pheny1]ethanone, 2-acety1-3-[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-6,6,9a-trimethylnaphtho[1,2-c]furan-3-yl]-2,5-cyclohexadiene-1,4-dione, 2-[(5aS,9aS)-4,5,5a,6,7,8,9,9a-octahydro-6,6,9a-trimethylnaphtho[1,2c]furan-3-yl]-3,6-dioxo-1,4-cyclohexadiene-1-carboxylic acid Me ester, and (-) - (2bS, 6aS, 7aS) -2b, 3, 4, 5, 6, 6a, 7, 7a-octahydro-11-hydroxy-2b, 6, 6trimethylbenzo[b] furo[2,3,4-mn]xanthene-12-carboxaldehyde.

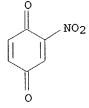
3958-76-7, 2-Nitro-1,4-benzoquinone IT

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and antiprotozoal activity of (euryfuryl) quinones (euryfuryl) hydroguinones)

3958-76-7 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2-nitro- (9CI) (CA INDEX NAME) CN



REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS 21 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 8 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2000:252240 HCAPLUS

DOCUMENT NUMBER:

132:280740

TITLE:

Antibacterial paper for safe food packaging

INVENTOR(S):

Hara, Kenichi

PATENT ASSIGNEE(S):

Daiko Seishi K. K., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2000110099	A2	20000418	JP 1998-281515	19981002
PRIC	RITY APPLN. INFO.:			JP 1998-281515	19981002
AB	The paper is wet la	id from	virgin pulp	and has been coated wi	th natural
	extract obtained fr	om bamb	oo based qui	none and tea based cate	chin.
IT	106-51-4D, Quinone,				
	RL: BUU (Biological	use, u	nclassified)	; BIOL (Biological stud	ly); USES
	(Uses)				
	(for manufacture	of ant	ibacterial p	aper for safe food pacl	kaging)
RN	106-51-4 HCAPLUS				
CN	2,5-Cyclohexadiene-	1,4-dio	ne (9CI) (C	A INDEX NAME)	

L25 ANSWER 9 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:440809 HCAPLUS

DOCUMENT NUMBER:

131:164556

TITLE:

Complexes of 2,5-dihydroxy-1,4-benzoquinone and

chloranilic acid with second and third row transition

elements

AUTHOR(S):

Mostafa, Sahar I.

CORPORATE SOURCE:

Department of Chemistry, Faculty of Science, Mansoura

University, Mansoura, Egypt

SOURCE:

Transition Metal Chemistry (Dordrecht, Netherlands)

(1999), 24(3), 306-310

CODEN: TMCHDN; ISSN: 0340-4285

PUBLISHER:

Kluwer Academic Publishers

DOCUMENT TYPE:

Journal

LANGUAGE:

English

The synthesis of new 2,5-dihydroxy-1,4-benzoquinone (H2DHBQ) and chloranilic acid (H2CA) complexes cis-[Mo2O5L2]2- (L = DHBQ, CA), [W2O5(DHBQ)2]2-, [WO2(CA)2]2-, trans-[UO2(DHBQ)]·H2O, and trans-[UO2(CA)2]2- is described. Raman, IR, 1H and 13C NMR spectra of the ligands and their complexes are reported and their structures discussed. The antimicrobial activity of the free ligands and several of the complexes was studied.

615-94-1, 2,5-Dihydroxy-1,4-benzoquinone IT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(antibacterial activity and reactant for preparation of transition metal dihydroxybenzoquinonato complexes)

615-94-1 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy- (9CI) (CA INDEX NAME) CN

REFERENCE COUNT:

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS 24 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 10 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1997:265584 HCAPLUS

DOCUMENT NUMBER:

126:248760

TITLE:

Bridged diphenyl compounds as drugs against parasitic

protozoa

INVENTOR(S):

Winter, Rolf Walter; Riscoe, Michael Kevin; Hinrichs,

David J.

PATENT ASSIGNEE(S):

Interlab Corporation, USA PCT Int. Appl., 35 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA'	TENT I	NO.			KINI	<b>o</b> 1	DATE		i	APPL	ICAT	I NOI	10.		D	ATE	
						-		<del>-</del>							-		
WO	9707	790			A1		19970	0306	I	WO 1	996-I	JS136	572		1:	99608	323
	W:	ΑL,	AM,	ΑT,	ΑU,	ΑZ,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	EE,
		ES,	FI,	GB,	GE,	HU,	ΙL,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LK,	LR,	LS,
		LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NΖ,	PL,	PT,	RO,	RU,	SD,
		SE,	SG,	SI,	SK,	ТJ,	TM,	TR,	TT,	UA,	UG,	US,	UZ,	VN,	AM,	ΑZ,	BY,
		KG,	KZ,	MD,	RU,	ТJ,	TM										
	RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,
		ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA		
AU	9668	589			<b>A</b> 1		19970	0319	i	AU 1	996-6	58589	9		1:	99608	323
PRIORIT	Y APPI	LN.	INFO	. :					Ţ	JS 1	995-5	52069	94	I	1	99508	328
									1	WO 1	996 - ા	JS136	572	V	1	99608	323
OTHER SO	OURCE	(S):			MARI	PAT	126:2	24876	50								

AΒ The synergistic combination of certain bridged di-Ph compds. [I; A = C(0), O, NH, S, S(0), SO2, C:C, NR, CX1X2; R, X1, X2 = H, OH, (halo)alkyl, (halo)alkylamino; R1-R10 = H, OH, halo, OAc, OMe, NH2, SO3-, N3, (halo)alkyl, alkylamino, aminoalkoxy, CO2X3; X3 = H, alkyl] with oxidants for the treatment of infectious diseases caused by protozoa is disclosed. Thus, the inhibition of growth of Plasmodium falciparum in vitro by rufigallol was potentiated 350-fold by 2,3,4,3',4',5'hexahydroxybenzophenone (exifone).

106-51-4, 2,5-Cyclohexadiene-1,4-dione, biological studies IT RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(bridged di-Ph compds. as drugs against parasitic protozoa)

RN106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) CN(CA INDEX NAME)

HCAPLUS COPYRIGHT 2004 ACS on STN L25 ANSWER 11 OF 36

ACCESSION NUMBER: 1995:646431 HCAPLUS

DOCUMENT NUMBER: 123:165058

TITLE: Fungitoxic compounds from the roots of tomato stock AUTHOR (S):

Nagaoka, Toshinori; Ohra, Junko; Yoshihara, Teruhiko;

Sakamura, Sadao

CORPORATE SOURCE: Fac. Appl. Biol. Sci., Hiroshima Univ.,

Higashihiroshima, 724, Japan

SOURCE: Nippon Shokubutsu Byori Gakkaiho (1995), 61(2), 103-8

CODEN: NSBGAM; ISSN: 0031-9473

DOCUMENT TYPE: Journal English LANGUAGE:

Fungitoxic compds. from the roots of tomato stocks, Taibyo Shinko Number 1, were determined as 4 unsatd. hydroxy fatty acids, (13S)-13-hydroxy-(9Z,11E)-9,11-octadecadienoic acid, 13-hydroxy-(9E,11E)-9,11-octadecadienoic acid, (9S) -9-hydroxy-(10E, 12Z) -10, 12-octadecadienoic acid and 9-hydroxy-(10E,12E)-10,12-octadecadienoic acid, a dicarboxylic acid (azelaic acid), a quinone (2,6-dimethoxy-p-benzoquinone) and 5 phenolic compds. (vanillin, syringaldehyde, p-hydroxybenzaldehyde, p-hydroxybenzoic acid, vanillic acid). It can be considered that the fungitoxic compds. related to resistance of the tomato stock against soil-borne disease were alkaloids, but not these universal compds. in plants.

IT530-55-2

> RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(fungitoxic compds. from roots of tomato stock)

RN 530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)

OMe O OMe

L25 ANSWER 12 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:604351 HCAPLUS

DOCUMENT NUMBER:

123:8036

TITLE:

Manufacture of antibacterial and antifungal substances from syringaldehyde with peroxidase and antibacterial

and antifungal agents containing the substances

INVENTOR(S): Kobayashi, Akio; Oguchi, Yasushi; Kanzaki, Hiroshi;

Kajama, Shinichiro; Kawazu, Kazuyoshi

PATENT ASSIGNEE(S):

SOURCE:

Kibun Shokuhin Kk, Japan

Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

LANGUAGE:

Patent Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		<b></b>		
JP 07076547	A2	19950320	JP 1993-223415	19930908
JP 3529814	B2	20040524		
PRIORITY APPLN. INFO.:			JP 1993-223415	19930908
CT				

OHC

AB Antibacterial and antifungal substances are manufactured by treatment of syringaldehyde (I) with peroxidase in the presence of H2O2. I was

IV

OMe

incubated with peroxidase and H2O2 at 25° and pH 5.8 for .apprx.3 h to manufacture a quinone II, a Ph ether III, and a biphenyl compound IV. II, III, and IV inhibited Escherichia coli with min. inhibitory concns. of 63, 500, and 500  $\mu$ g/mL, resp.

IT530-55-2P

RL: BAC (Biological activity or effector, except adverse); BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)

(manufacture of antibacterial and antifungal compds. with peroxidase and H2O2 from syringaldehyde)

530-55-2 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME) CN

OMe

L25 ANSWER 13 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:451619 HCAPLUS

DOCUMENT NUMBER: 121:51619

TITLE: Expert-system comparison of structural determinants of

chemical toxicity to environmental bacteria

AUTHOR (S): Pangrekar, Jyotsna; Klopman, Gilles; Rosenkranz,

Herbert S.

CORPORATE SOURCE: Grad. Sch. of Public Health, Univ. Pittsburgh,

Pittsburgh, PA, 15261, USA

SOURCE: Environmental Toxicology and Chemistry (1994), 13(6),

979-1001

CODEN: ETOCDK; ISSN: 0730-7268

DOCUMENT TYPE:

Journal LANGUAGE: English

The CASE (computer automated structure evaluation) structure-activity relational expert system was used to analyze the toxicity of a database of chemical sets to environmental bacteria (aerobic heterotrophs, nitrosomonas, methanogens, and photobacteria [Microtex test]). The anal. revealed that the data sets related to each of the antimicrobial activities, albeit containing a relatively small number of chems., are characterized by structural determinants significantly associated with the probability of antimicrobial activity, as well as with antibacterial potency. Although three were a number of 'similarities among the structural determinants associated with each of these antimicrobial activities, there were also features unique to each assay that presumably reflect species-specific targets of bactericidal activity. Overall the assay for antimethanogenic activity appears to be the most informative as well as the one most predictive of the activity in the other three assays.

IT 82-68-8, Pentachloronitrobenzene 106-51-4,

1,4-Benzoquinone, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to environmental bacteria, expert system in study of)

RN 82-68-8 HCAPLUS

CN Benzene, pentachloronitro- (8CI, 9CI) (CA INDEX NAME)

$$C1$$
 $C1$ 
 $C1$ 
 $C1$ 
 $C1$ 

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L25 ANSWER 14 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1994:210628 HCAPLUS

DOCUMENT NUMBER:

120:210628

TITLE:

Detection of herbicides via a bacterial photoreaction

center and bacterial luciferase

AUTHOR (S):

Jockers, Ralf; Schmid, Rolf D.

CORPORATE SOURCE:

Proj. Group Biosens., GBF--Ges. Biotechnol. Forsch.

mbH, Braunschweig, D(W)-3300, Germany

SOURCE:

Biosensors & Bioelectronics (1993), 8(6), 281-9

CODEN: BBIOE4; ISSN: 0956-5663

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB A new detection principle for ligands (photosystem-II herbicides) based on bacterial luciferase as the detection system is presented. The dependency of luciferase on long-chain aliphatic aldehydes was used. The requirements for such a system are investigated. Studies were made of the binding properties of artificial aldehydes to the QB-binding site of photoreaction centers from the phototrophic bacteria Rhodobacter sphaeroides and substrate properties for bacterial luciferase from Photobacterium fischeri of various artificial aldehydes.

IT 106-51-4, 1,4-Benzoquinone, biological studies 605-94-7,

Ubiquinone 0

RL: PROC (Process)

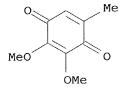
(binding of, to QB site of bacterial photoreaction center)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)



ANSWER 15 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1994:25511 HCAPLUS

DOCUMENT NUMBER:

120:25511

TITLE:

Naturally occurring antidotes against benzimidazole

fungicides

AUTHOR(S):

Tahara, Satoshi; Matsukura, Yumiko; Katsuta, Hiroyuki;

Mizutani, Junya

CORPORATE SOURCE:

Fac. Agric., Hokkaido Univ., Sapporo, 060, Japan

SOURCE:

Zeitschrift fuer Naturforschung, C: Journal of

Biosciences (1993), 48(9-10), 757-65

CODEN: ZNCBDA; ISSN: 0341-0382

DOCUMENT TYPE:

Journal

LANGUAGE:

English

TLC bioautog. using precoated glass thin-layer plates impregnated with benomyl or carbendazim (MBC), and Cladosporium herbarum as a test fungus, was evaluated as a facile way to detect plant secondary metabolites antidoting against benzimidazole fungicides. In addition to emodin and  $\alpha$ -tocopherol from Polygonum sachalinense, three phenolics, 3,5-dihydroxy-4-methylstilbene and 5-methoxy-6,7-methylenedioxyflavone from P. lapathifolium and 2,6-dimethoxybenzoquinone from P. thunbergii, were isolated and characterized as new benzimidazole antidotes. Emodin exhibited the antidoting activity not only against benomyl but also against MBC, thiabendazole, thiophanate-Me and nocodazole. Furthermore, emodin showed antidoting activity against MBC in the wild-type Neurospora crassa and against diethofencarb in the mutant of N. crassa resistant to benzimidazole fungicides but highly susceptible to diethofencarb.

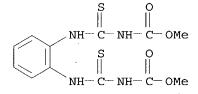
23564-05-8, Thiophanate-methyl IT

RL: BIOL (Biological study)

(antidotes against, emodin as)

RN23564-05-8 HCAPLUS

CN Carbamic acid, [1,2-phenylenebis(iminocarbonothioyl)]bis-, dimethyl ester (9CI) (CA INDEX NAME)



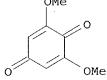
IT 530-55-2

RL: BIOL (Biological study)

(benzimidazole fungicide antidote, from Polygonum thunbergii)

RN530-55-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)



L25 ANSWER 16 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:555979 HCAPLUS

DOCUMENT NUMBER:

119:155979

TITLE:

Inhibition of Mucor rouxii growth by synthetic

substances

AUTHOR (S):

Sabanero, Myrna; Rojas, Emma; Torres, Veronica;

Farfan, Norberto; Contreras, Rosalinda

CORPORATE SOURCE:

Fac. Quim., Univ. Guanajuato, Mex.

SOURCE:

Revista Latinoamericana de Microbiologia (1991),

33(4), 297-303

CODEN: RLMIAA; ISSN: 0034-9771

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Micor rouxii cells were used to examine the possible antimycotic activities of 4 substances: phenolamines, phenylenediamine and quinone. These substances are original structures recently synthesized. Assays in plates showed that 10-2 M of phenolamines and phenylenediamines give rise to halos of growth inhibition. Assays in liquid media using 10-4 M of substances showed 100% inhibition of spore germination. Specifically, the phenylenediamine showed 49% inhibition on development of mycelium. In these cells the calcofluor distribution changes, suggesting alterations in cell wall. No inhibition of growth was found using the quinone. The activity for substances were evaluated using standard antifungal benomyl. On this basis, phenylendiamine is antimycotically active. The mechanism of action is not presently known.

IT 106-51-4P, Quinone, preparation

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and fungicidal activity of)

106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

RN

CN

L25 ANSWER 17 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:508064 HCAPLUS

DOCUMENT NUMBER:

115:108064

TITLE:

A database of chemical toxicity to environmental bacteria and its use in interspecies comparisons and

correlations

AUTHOR(S):

Blum, Diane J. W.; Speece, R. E.

CORPORATE SOURCE:

Bala Cynwyd, PA, 19004, USA

SOURCE:

Research Journal of the Water Pollution Control

Federation (1991), 63(3), 198-207 CODEN: RJWFE7; ISSN: 1047-7624 DOCUMENT TYPE:

Journal

LANGUAGE:

English

This research assayed the toxicity of 50-100 chems. to each of 3 bacterial groups: aerobic heterotrophs, Nitrosomonas, and methanogens. Chems. tested comprise important environmental pollutants such as chlorinated aliphatic hydrocarbons and halogenated and other substituted benzenes and

IT

RN

CN

RN

CN

Toxicity data were obtained from the literature for fathead minnows and for the Microtox test for comparison with author's bacterial Aerobic heterotrophs and methanogens showed similar sensitivities to toxicants, with the exception of an enhanced susceptibility of methanogens to chlorinated aliphatic hydrocarbons and alcs. Nitrosomonas, Microtox, and the fathead minnow showed similar sensitivities as one another, which were one order of magnitude greater than the sensitivities of the aerobic heterotrophs and methanogens. Correlations among the toxicities to different organisms allow predictions of a chemical toxicity to one organism to be made based on the toxicity of that chemical to a different organism. Excellent correlations were found between chemical toxicities to

the aerobic heterotrophs, methanogesn (with chlorinated aliphatic hydrocarbons omitted), and fathead minnows. Good correlations were found between Microtox and each of the other bacteria and the fathead minnow.

82-68-8 106-51-4, 1,4-Benzoquinone, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of, to environmental bacteria, species in relation to)

82-68-8 HCAPLUS

Benzene, pentachloronitro- (8CI, 9CI) (CA INDEX NAME)

$$C1$$
 $N0_2$ 
 $C1$ 
 $C1$ 

106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

TITLE:

SOURCE:

L25 ANSWER 18 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:22693 HCAPLUS

DOCUMENT NUMBER:

114:22693

INVENTOR(S):

Microbicidal agents containing benzoquinones for foods

Nishina, Atsuro; Ito, Masaji

PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 2 pp.

Nippon Oil and Fats Co., Ltd., Japan

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

## Pryor 10\_003465

KIND DATE APPLICATION NO. PATENT NO. 19900810 19890201 JP 02202804 A2 JP 1989-20796 JP 1989-20796 19890201 PRIORITY APPLN. INFO.: Microbicidal agents contain benzoquinones as effective components. The benzoquinones are safe and inexpensive, have a broad spectrum of activity, and are useful for foods. Min. inhibitory concentration values of methyl-p-benzoquinone, 2,3-dimethoxy-5-methyl-p-benzoquinone, and 2,6-dimethoxy-p-benzoquinone against various bacteria and fungi are given. IT530-55-2, 2,6-Dimethoxy-p-benzoquinone 553-97-9, Methyl-p-benzoquinone 605-94-7, 2,3-Dimethoxy-5-methyl-pbenzoguinone RL: BIOL (Biological study) (bactericide and function, for foods) 530-55-2 HCAPLUS RN CN2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy- (9CI) (CA INDEX NAME)

OMe O

RN 553-97-9 HCAPLUS

OMe

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)

Me

RN 605-94-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl- (9CI) (CA INDEX NAME)

L25 ANSWER 19 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:402345 HCAPLUS

DOCUMENT NUMBER: 109:2345

TITLE: In vitro evaluation of some natural products for their

fungitoxicity

AUTHOR(S): Dube, S.; Shukla, H. S.; Tripathi, S. C.

CORPORATE SOURCE: Dep. Bot., Univ. Gorakhpur, Gorakhpur, 273009, India

SOURCE: Pesticides (1988), 22(3), 11-12

CODEN: PSTDAN; ISSN: 0031-6148

DOCUMENT TYPE:

Journal English

LANGUAGE:

Of 18 natural products, benzoquinone, m-chloroaniline, and o-cresol were the most effective against Aspergillus flavus. At 500 ppm they inhibited mycelial growth by 90%. At 700 ppm, these compds., as well as camphor, catechol, and p- and m-cresol, totally suppressed the growth. Me imparted higher effectiveness to the phenol ring than did either NH2 or COOH. Amino group at the phenol ring was more effective at ortho than at the para or meta positions. Two or more OH groups also increased the antifungal potency.

TT 106-51-4, biological studies RL: BIOL (Biological study)

(fungitoxicity of)

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

HCAPLUS COPYRIGHT 2004 ACS on STN L25 ANSWER 20 OF 36

ACCESSION NUMBER:

1986:507995 HCAPLUS

DOCUMENT NUMBER:

105:107995

TITLE:

Respiratory inhibition by the antifungal benzoquinone,

AUTHOR(S):

2-hydroxy-6-methoxy-3,5-dimethyl-1,4-benzoquinone Haraguchi, Hiroyuki; Soga, Osamu; Taniguchi, Makoto

CORPORATE SOURCE:

Fac. Sci., Osaka City Univ., Osaka, 558, Japan

SOURCE:

Agricultural and Biological Chemistry (1986), 50(7),

1905-7

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE:

LANGUAGE:

Journal

GΙ

English

Me OH OMe Т Me

The title antifungal compound I [76186-46-4] lowered the AB respiratory-control but not the ADP/O ratio of rat liver mitochondria (used instead of the more unstable fungal mitochondria) incubated with  $\alpha$ -ketoglutarate and succinate as the respiratory substrates. I depressed the state-3 but not state-4 respiration rate in 2,4-dimitrophenol-uncoupled mitochondria. Also, I inhibited succinate-[9028-10-8] and NADH-cytochrome C reductase [9027-14-9]. Thus, the site of respiration inhibition by I appears to be in the electron-transport system. The effect of I on mitochondria may be related to its antifungal action. The antimicrobial potency of I against several bacteria

and fungi in vitro was also studied.

L25 ANSWER 21 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1985:58267 HCAPLUS

DOCUMENT NUMBER:

102:58267

TITLE:

Mediator function of biologically active n-type quinones in a peroxidase enzymic reaction initiated

electrochemically

Shapovalov, V. A.

CORPORATE SOURCE:

Khar'k. Gos. Farm. Inst., Kharkov, USSR Elektrokhimiya (1984), 20(10), 1383-5

CODEN: ELKKAX; ISSN: 0424-8570

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

AUTHOR(S):

Russian

The electrochem. reduction of quinone derivs. during the reaction of peroxidase with H2O2 was investigated, and the physiol. effectiveness of the derivs. as fungicides was compared to their ability to stimulate the peroxidase reaction. The time for conversion of 1/2 of the available H2O2 by the enzyme in the presence of the quinone derivs.  $(\tau 1/2)$  correlated well with their fungicidal activities. Furthermore, the limiting current for electrochem. reduction of the quinones in the presence of enzyme also correlated with the  $\tau 1/2$ . Thus, the electrochem. reduction of quinones in the presence of peroxidase may constitute a screening procedure for the fungicidal activity of quinones.

106-51-4, reactions 106-51-4D, derivs. ТТ

RL: RCT (Reactant); RACT (Reactant or reagent)

(electrochem. reduction of, in peroxidase presence, fungicidal

activity in relation to)

106-51-4 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L25 ANSWER 22 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1979:503756 HCAPLUS

DOCUMENT NUMBER:

91:103756

TITLE: INVENTOR(S):

SOURCE:

Methylbenzoquinone fungicides Watanabe, Yoshihachi; Iwao, Toru Shionogi and Co., Ltd., Japan

PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 2 pp. CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

## Pryor 10 003465

PATENT NO.	KIND .	DATE	APPLICATION NO.	DATE
JP 54067027	A2	19790530	JP 1977-132920	19771104
PRIORITY APPLN. INFO.:			JP 1977-132920	19771104
GI				

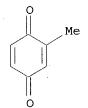
o Ne

AB 2-Methyl-1,4-benzoquinone (I) [553-97-9] controls soil phytopathogens. Thus, 1000 ppm I controlled Phythium aphanidematum, Rhizoctonia solani, and Fusarium oxysporum in soil.

TT 553-97-9
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicides) RN 553-97-9 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



L25 ANSWER 23 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1978:501628 HCAPLUS

DOCUMENT NUMBER:

89:101628

TITLE:

AB

In vitro effect of some phenols, quinones and growth hormones on the fungal pathogens causing wilt of gram

(Cicer arietinum L.)

AUTHOR(S):

Mathur, Sunila; Chauhan, S. K.

CORPORATE SOURCE: SOURCE:

Sch. Stud. Bot., Vikram Univ., Ujjain, India Proceedings of the National Academy of Sciences,

India, Section B: Biological Sciences (1976), 46(4),

491-4

CODEN: PAIBA6; ISSN: 0369-8211

DOCUMENT TYPE:

Journal English

LANGUAGE:

PhOH [108-95-2], catechol [120-80-9], pyrogallol [87-66-1], benzoquinone [**106-51-4**], IAA [87-51-4], 2,4-D [94-75-7], 2-naphthoxyacetic acid [120-23-0], NAA [86-87-3], biotin [58-85-5],

thiamin [59-43-8], and inositol [87-89-8] were tested for their

fungicidal properties against Fusarium oxysporum, Rhizotonia
solani and Sclerotium rolfsii, causing wilt of gram (C. arietinum), at 10,
50, and 100 ppm. These compds. caused different effects on the growth of
the pathogens as revealed by the difference in colony diams., dry mycelial

weight and percentage germination of spores (only in the case of Fusarium). Benzoquinone, PhOH, catechol, pyrogallol, thiamin, and IAA were effective against F. oxysporum and catechol and IAA against R. solani and S. rolfsii.

106-51-4, biological studies IT

> RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicide, for gram wilt control)

106-51-4 HCAPLUS RN

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L25 ANSWER 24 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:578837 HCAPLUS

87:178837 DOCUMENT NUMBER:

The effect on fungal growth of some TITLE:

Journal

2,5-dihydroxy-1,4-benzoquinones

Brewer, D.; Maass, W. S. G.; Taylor, A. AUTHOR (S):

Natl. Res. Counc. Canada, Halifax, NS, Can. CORPORATE SOURCE:

Canadian Journal of Microbiology (1977), 23(7), 845-51 SOURCE:

CODEN: CJMIAZ; ISSN: 0008-4166

DOCUMENT TYPE:

English LANGUAGE:

GI

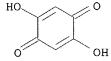
2,5-Dihydroxy-1,4-benzoquinones decreased vegetative growth and inhibited AR spore germination of 12 species of fungi belonging to 6 diverse genera. The nature of the substituents at the 3 and 6 positions of the quinone ring affected their growth-inhibitory properties; generally those substituents of lower polarity inhibited growth at lower concns. As in the case of cochliodinol (I) [11051-88-0], chemical modification of the quinone group, or the hydroxyl groups of the quinone ring, in compds. of the polyporic acid series, also led to loss of biol. activity. IT 615-94-1D, derivs.

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicidal activity of)

615-94-1 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy- (9CI) (CA INDEX NAME) CN



L25 ANSWER 25 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:414559 HCAPLUS

DOCUMENT NUMBER: 85:14559

TITLE: Studies on fungal products. Part IV. Isolation of

oospolactone as the antifungal principle of

Gloeophyllum sepiarium

AUTHOR(S): Nakajima, Shoichi; Kawai, Kenichi; Yamada, Shizue;

Sawai, Yuko

CORPORATE SOURCE: Hoshi Coll. Pharm., Tokyo, Japan

SOURCE: Agricultural and Biological Chemistry (1976), 40(4),

811-12

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal LANGUAGE: English

LANGUAGE: English
AB Oospolactone (3,4-dimethyl-8-hydroxyisocoumarin) [1570-27-0], isolated

from G. sepiarum cultures, was active against a wide variety of **fungi.** Along with oospolactone, 2,5-dimethoxy-p-benzoquinone [ **3117-03-1**], methyl sulphrenate [19683-37-5], and ergosteryl

palmitate [3992-98-1] were isolated.

L25 ANSWER 26 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:116867 HCAPLUS

DOCUMENT NUMBER: 84:116867

TITLE: Fungitoxicity and insecticide synergism of

monothioquinol phosphate esters and related compounds

AUTHOR(S): Eto, Morifusa; Hashimoto, Yasuaki; Ozaki, Kozaburo;

Kassai, Tatsuo; Sasaki, Yoshitaka

CORPORATE SOURCE: Dep. Agric. Chem., Kyushu Univ., Fukuoka, Japan

SOURCE: Bochu Kagaku (1975), 40(3), 110-17

CODEN: BOCKAF; ISSN: 0006-5420

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Of O-Et S,S-di-Ph phosphorodithioate [17109-49-8], 4 phosphorothioates (EtO)2P(O)SC6H4R-4 (R = OH, OMe, OCO2Et, or Me), and 9 phosphates

(R10)2P(0)OR2 (R1 = Et or Ph, R2 = substituted Ph) synthesized, only the phosphorothioates and the phosphorodithioate showed fungitoxic activity against Aspergillus niger, in vitro. Some hydrolysis products, such as Ph disulfide [882-33-7] and p-hydroxythiophenol [637-89-8] were more

fungitoxic than the parent esters. There was a correlation between the fungitoxic activity, and the lipophilic character, as expressed by the

partition coefficient, for some of the compds. None of the compds. inhibited at 5 + 10-4M, the respiration of A. niger, whereas some oxidized

derivs. of the hydrolysis products, such as inhibitory had a strong

inhibtory activity. Tri-Ph phosphate [115-86-6] and di-Et S-ethoxycarbonyloxyphenyl phosphorothioate [40249-48-7] synergized the

insecticidal activity of malathion [121-75-5] against

malathion-resistant strain of Laodelphax striatellus. The

phosphorothioates synergized malathion much more than did tri-Ph phosphate against the green rice leafhopper (Nephotettix cincticeps). Tri-Ph

phosphate, di-Et 4-hydroxyphenyl phosphate [13953-88-3] and 0,0-di-Et S-ethoxycarbonyloxyphenyl phosphorothioate synergized the insecticidal

activity of carbaryl [63-25-2] against the tobacco cutworm (Prodenia litura), but less than did piperonyl butoxide.

106-51-4, biological studies

ΤТ

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicidal activity of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

IT 63-25-2 121-75-5

RL: BIOL (Biological study)

(insecticidal synergism with, by phosphates and phosphorothiolates)

RN 63-25-2 HCAPLUS

CN 1-Naphthalenol, methylcarbamate (9CI) (CA INDEX NAME)

RN 121-75-5 HCAPLUS

CN Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & S \\ \parallel \\ S-P-OMe \\ O & \mid & O\\ OMe & \mid & O\\ EtO-C-CH-CH_2-C-OEt \end{array}$$

L25 ANSWER 27 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1964:93975 HCAPLUS

DOCUMENT NUMBER:

60:93975

ORIGINAL REFERENCE NO.:

60:16440c

Journal

TITLE:

Quinone as a fungicide. The history of its

investigation and a view of its mode of action

AUTHOR(S):

Braune, Wolfram

CORPORATE SOURCE:

Friedrich-Schiller Univ., Jena, Germany

SOURCE:

Zentralblatt fuer Bakteriologie, Parasitenkunde, Infektionskrankheiten und Hygiene, Abteilung 2,

Naturwissenschaftliche: Allgemeine,

Landwirtschaftliche und Technische Mikrobiologie

(1964), 117(4), 412-24

CODEN: ZBPIA9; ISSN: 0044-4057

DOCUMENT TYPE:

LANGUAGE: Unavailable

AB A review with many references.

IT 106-51-4, p-Benzoquinone (fungicidal action of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L25 ANSWER 28 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1960:104762 HCAPLUS

DOCUMENT NUMBER: 54:104762
ORIGINAL REFERENCE NO.: 54:19969a-c

TITLE: The effects of benzothiazole derivatives and some

others upon Candida in vitro AUTHOR(S): Toda, Tadao; Tokunaga, Toru

CORPORATE SOURCE: Univ. Kyushu

SOURCE: Chemotherapy (Tokyo) (1959), 7, 332-5

CODEN: NKRZAZ; ISSN: 0009-3165

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

The growth-inhibitory activity toward Candida albicans, C. krusei, C. guilliermondi and several bacterial strains was examined in vitro of 6-carboxy-, 6-ethoxycarbonyl-, 6-carboxymethoxy-, 6-cyano-, 4,7-dichloro-6-cyano-, 4,7-dichloro-6-carboxy-, 6-carbamoyl-, and the HCl salt of 6-hydrazino carbonyl-2-methylbenzothiazole, 2-methylbenzothiazole-6-carbonylhydrazones of benzoquinone, 3-chlorobenzoquinone, quinoxime and 2-isopropyl-5-methylquinoxime, 6-methyl- and 6-ethoxycarbonyl-2-aminobenzothiazole, 2-acetamido-6-methyl-benzothiazole, monochlorobenzoquinone, 2,5-dichloro-4-thiocyanatoaniline (I), bis(2,5-dichloro-4-aminophenyl) disulfide, Et 3-thiocyanato-4-aminobenzoate, and nitrosothymol. All of benzothiazole derivs. were not so effective, but I had a high growth-inhibitory power against not only

Candida, but also bacteria generally. I was highly bacteriostatic against Mycobacterium tuberculosis including streptomycin and isonicotinoyl hydrazide (II)-resistant strains. Its acute toxicity in mice was much lower than II.

IT 106-51-4, p-Benzoquinone

(hydrazones with 2-methyl-6-benzothiazolecarboxylic acid hydrazide, bactericidal and fungicidal action of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L25 ANSWER 29 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1958:16486 HCAPLUS

DOCUMENT NUMBER: 52:16486
ORIGINAL REFERENCE NO.: 52:3014d-f

TITLE: Effects of some phenols and quinones on growth in

vitro of Verticillium albo-atrum

## Pryor 10 003465

AUTHOR(S):

LeTourneau, Duane; McLean, John G.; Guthrie, James W.

CORPORATE SOURCE:

Idaho Agr. Expt. Sta., Moscow Phytopathology (1957), 47, 502-6 CODEN: PHYTAJ; ISSN: 0031-949X

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

Unavailable

The effects of 13 phenols and phenolic acids and 4 quinones on the growth in liquid medium of V. albo-atrum were determined Of 3 isomeric dihydroxybenzenes, catechol (I) was most inhibitory. Replacement of an OH group with a COOH group or the introduction of a COOH group on the ring decreased the effectiveness of I. Pyrogallol was the most toxic phenolic compound tested. The quinones were generally more inhibitory than the phenols. 1,4-Naphthoquinone was more inhibitory than 1,4-benzoquinone, and chlorination of the quinones increased their inhibitory action. 2,3-Dichloro-1,4-naphthoquinone caused appreciable growth inhibition at a concentration of 10-6M.

106-51-4, p-Benzoquinone IT

(as fungicide for Verticillium albo-atrum)

RN106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

L25 ANSWER 30 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1955:62269 HCAPLUS

DOCUMENT NUMBER:

49:62269

ORIGINAL REFERENCE NO.: 49:11947a-c

TITLE:

Fungicidal preparations

INVENTOR(S):

Tjepkema, Jacobus J.; Montagne, Johannes Th. W.

PATENT ASSIGNEE(S):

.N. V. de Bataafsche Petroleum Maatschappij

DOCUMENT TYPE:

Patent

LANGUAGE:

Unavailable

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE -----\_\_\_\_\_\_

NL 76833

19541215 NL

New and valuable fungicides have been found in 1,4-benzoquinones and AB 1,4-naphthoguinones where the first type carries 2 or 4 alkylthio groups, the latter 2 alkylthio groups. They are used in the form of aqueous emulsions of solns. of the compds. in hydrocarbon oils. Because of their good solubility in mineral oil they can be applied by the method of low-volume spraying. E.g. for 2,3-bis(isopropylthio)-1,4-naphthoquinone the solubility is 3% and the L.D.50 is 2.5 p.p.m.; for 2,3,5,6-tetrakis(isoamylthio)-1,4-benzoquinone the solubility is 25% and the L.D.50 is 20 p.p.m., as measured by the "Slide germination method".

106-51-4, p-Benzoquinone IT

(derivs., for fungicides)

RN106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN



L25 ANSWER 31 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1955:30526 HCAPLUS

DOCUMENT NUMBER: 49:30526 ORIGINAL REFERENCE NO.: 49:5848h

TITLE: Preparation of microbiologically resistant wool by

chemical modification. VI. Benzoquinone, ninhydrin,

and heavy metal salts

AUTHOR(S): Zahn, Helmut; Wurz, Albrecht; Rauchle, Adolf

CORPORATE SOURCE: Univ. Heidelberg, Germany

SOURCE: Textile Research J. (1955), 25, 120-4

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB The beneficial effects of these compds. are noted. Treatment with bis(chloromethyl)benzene protects against attack by bacteria, moths, and

alkali. Possibilities for com. applications are suggested.

IT 106-51-4, p-Benzoquinone

(wool proofing against bacteria and fungi by)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L25 ANSWER 32 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1954:40456 HCAPLUS

DOCUMENT NUMBER: 48:40456
ORIGINAL REFERENCE NO.: 48:7243f-h

TITLE: Fungicidal action. II. Constitution of benzenoid and

quinonoid compounds in relation to fungitoxicity and inhibition of amino- and sulfhydryl-dependent enzymes

AUTHOR(S): Owens, Robert G.

SOURCE: Contributions from Boyce Thompson Institute (1953),

17, 273-82

CODEN: CBTIAE; ISSN: 0006-8543

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

cf. McNew and Burchfield, C.A. 46, 11543a. The inhibition of pancreatic and malt amylases was compared with the ED50 value against Alternaria oleracea and Monilinia fructicola. Inhibitory effects and fungicidal effects were correlated with durene, 4-nitroveratrole, veratrole, hydroquinone dimethyl ether, hydroquinone diethyl ether, guaiacol, resorcinol, catechol, di-tert-amylhydroquinone, toluhydroquinone, 2,5-dichlorohydroquinone, p-benzoquinone, tolu-p-benzoquinone, chloranilic acid, 2,5-dichloroquinone, 2,6-dichloroquinone, and 2,6-dichloroquinone chloroimide. 2,4-Dichlorotoluene, 3,4-dichlorotoluene, hydroquinone monomethyl ether, p-xyloquinone, 1,4-naphthoquinone, 2-methyl-1,4-naphthoquinone, and 2,3-dichloro-1,4-naphthoquinone were more active against the fungi than against the enzymes. Hydroquinone, tetrachloro-p-benzoquinone, and 1,2-naphthoquinone were more active

against the enzymes.

137-18-8, Phlorone 553-97-9, p-Toluquinone IT (fungitoxicity of and enzyme inhibition by)

137-18-8 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2,5-dimethyl- (9CI) (CA INDEX NAME) CN

553-97-9 HCAPLUS RN

2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME) CN

IT 106-51-4, p-Benzoquinone

(fungitoxicity of, and enzyme inhibition by)

106-51-4 HCAPLUS RN

CN2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)

L25 ANSWER 33 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1953:7439 HCAPLUS

DOCUMENT NUMBER:

47:7439

ORIGINAL REFERENCE NO.:

47:1326c-e

TITLE:

Fungicidal and insecticidal preparations containing

halogenated duroquinone

INVENTOR(S):

Schmidl, Albert U.

PATENT ASSIGNEE(S):

Standard Oil Development Co.

DOCUMENT TYPE:

Patent

LANGUAGE:

Unavailable

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_\_\_ US 2615827 19521028 US

Halogenation of duroquinone (I) in the presence of light and (or) a halogen AB carrier is controlled until I contains an average of more than 50% by weight of halogen on the nonaromatic C atoms. When the slide germination method is used, a solution of 0.001-0.0001 weight % of chlorinated duroquinone (II) containing 54.5% by weight of Cl allowed only 50% germination to Alternaria solani and

Sclerotinia fructiola. Immersion of a milk-weed bug for 2 min. in a 0.25 weight % suspension of II produces 100% mortality. The same treatment produces 30% mortality of the German roach. Injection of 0.5 mg. of II per g. of body weight into the blood stream of the American roach results in 100% mortality. When the Nelson drop test is used, a suspension of II results in 95% mortality of the housefly. Halogenated I exhibits no phytotoxicity on coleus.

527-17-3, p-Benzoquinone, tetramethyl-IT

(chlorinated, fungicides and insecticides from)

RN 527-17-3 HCAPLUS

CN2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)

L25 ANSWER 34 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

1952:52712 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 46:52712 ORIGINAL REFERENCE NO.: 46:8779c-g

TITLE:

Antiseptics for foods. LI

AUTHOR (S): Fujikawa, Fukujiro; Tokuoka, Akimasa; Takimura,

Miyoko; Miura, Kazuko

CORPORATE SOURCE:

Kyoto Coll. Pharm.

Yakugaku Zasshi (1952), 72, 518-20 SOURCE:

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE:

LANGUAGE: Unavailable

cf. C.A. 46, 1714c. -Quinone; p-0:C6H4:NNHC(:NH)NH2.HNO3;

p-C6H4[:NNHC(:NH)NH2.HNO3]2; p-toluquinone; 2,4-

Journal

Me(O:)C6H3:NNHC(:NH)NH2.HNO3; 2,1,4-MeC6H3[:NNHC(:NH)NH2.HNO3]2;

 $\alpha\text{-naphthoquinone}$  (I); 1,4-0:C10H6:NNHC(:NH)NH2.HNO3;

1,4-C10H6[:NNHC(:NH)NH2.HNO3]2; thymoquinone and its

diaminoquanylhydrazone nitrate; 2-methyl-5-methoxyquinone; anthraquinone derivs. including chrysophanol purpurin, anthrachrysone, rufigallic acid, emodic acid, and endocrocin; α-benzildioxime; salicylaldoxime;

o-HOC9H6N (II); PhN(NO)ONH4; and phenanthraquinone (III) were tested for mold-preventing action in soy sauce. I and II showed about the same

degree of activity as that of p-HOC6H4CO2Pr used as a control; III

prevented the growth of mold for 42.5 days at the concentration of 0.001%, 51.5 days at 0.003%, and 77 days at 0.005% in contrast to the control which

prevented the growth of mold for 77 days at the concentration of 0.01%. Other

compds. were ineffective.

106-51-4, p-Benzoquinone 553-97-9, p-Toluquinone IT

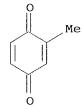
(as fungicides in soy sauce)

RN106-51-4 HCAPLUS

2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME) CN

RN 553-97-9 HCAPLUS

2,5-Cyclohexadiene-1,4-dione, 2-methyl- (9CI) (CA INDEX NAME)



CN

L25 ANSWER 35 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1952:23744 HCAPLUS

DOCUMENT NUMBER: 46:23744
ORIGINAL REFERENCE NO.: 46:4057f-h

TITLE: Fungistatic potencies of some fluorinated p-quinones

AUTHOR(S): Tehon, Leo R.

CORPORATE SOURCE: Illinois State Nat. History Survey, Urbana

SOURCE: Science (Washington, DC, United States) (1951), 114,

663-4

CODEN: SCIEAS; ISSN: 0036-8075

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

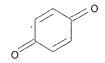
AB In order to compare the effects of fluorinated quinones with those of quinones containing other halogens, bioassays according to the method of Peterson (Phytopathology 31, 1108(1941)) were carried out on 2-fluoro-1, 4-quinone, 2, 5-difluoro-1, 4-quinone (I), 2-fluoro-5-chloro-1, 4-quinone, 2-fluoro-5-bromo-1, 4-quinone, and 2-fluoro-5-methyl-1, 4-quinone (II). The test fungus presumably was a subtransplant of the strain of Macrosporium sarcinaeforme used by McCallan (Cornell University Agr. Experiment Sta., Mem. Number 128). Readings of spore germination were made after incubating 20 hrs., averaging the values obtained from 4 replicates. Most effective in preventing germination of spores was I. Methylation, as in II, appeared to diminish toxicity appreciably. In general the effective dosages for fluorinated quinones are remarkably low.

IT 106-51-4, p-Benzoquinone

(fluorinated derivs., fungistatic potencies of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



L25 ANSWER 36 OF 36 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1951:22830 HCAPLUS

DOCUMENT NUMBER: 45:22830
ORIGINAL REFERENCE NO.: 45:4002e-f

TITLE: Antifungal agents and antimycotic therapy

AUTHOR(S): Stedman, Russell L.

CORPORATE SOURCE: McNeil Labs., Inc., Philadelphia, PA

SOURCE: Bull. Natl. Formulary Comm. (1950), 18, 153-75

DOCUMENT TYPE: Journal

# Pryor 10\_003465

LANGUAGE:

Unavailable

AB A review dealing with the following groups of therapeutic agents: fatty acids, older remedies consisting of dyes, organic acids, inorg. salts, and halogens, antibiotics, hormones, newer fungal agents including aldehyde, ketone, and ether derivs., phenol and cresol derivs., quinone, pyridine, quinoline, and thio derivs., chelating agents, and miscellaneous agents. 153 references.

IT 106-51-4, p-Benzoquinone

(derivs., fungicidal action of)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)